

**3.3.1 Number of research papers published per teacher in the Journals notified on UGC website during the last five years (2018-2023)**

Sl. No.	Title of paper	Name of the author/s	Department of the teacher	Name of journal	Year of publication	ISSN number	Link to the recognition in UGC enlistment of the Journal /Digital Object Identifier (doi) number		
							Link to website of the Journal	Link to article / paper / abstract of the article	Is it listed in UGC Care list
1.	Development of a new fluorescence ratiometric switch for endogenous hypochlorite detection in monocytes of diabetic subjects by dye release method. <i>Tetrahedron Letters</i> , 59(12), Pgs: 1130 – 1135.	Das,S.; <b>Aich,K.</b> ;Patra,L.; Ghoshal,K.;Gharami,S.; Bhattacharyya,M.;Mondal, T. K.	Chemistry	Tetrahedron Letters	2018	0040-4039/1873-3581(online)	<a href="https://www.sciencedirect.com/science/article/abs/pii/S0040403918301928">https://www.sciencedirect.com/science/article/abs/pii/S0040403918301928</a>	<a href="https://doi.org/10.1016/j.tetlet.2018.02.023">https://doi.org/10.1016/j.tetlet.2018.02.023</a>	YES
2.	Detection and discrimination of Zn <sup>2+</sup> and Hg <sup>2+</sup> using a single molecular fluorescent probe. <i>New Journal of Chemistry</i> , 42(11), pgs: 8646 – 8652.	Gharami,S.; <b>Aich,K.</b> ;Patra,L.;Mondal, T. K.	Chemistry	New Journal of Chemistry	2018	1144-0546/1369-9261 (online)	<a href="https://pubs.rsc.org/en/content/article/anding/2018/nj/c8nj01212a">https://pubs.rsc.org/en/content/article/anding/2018/nj/c8nj01212a</a>	<a href="https://doi.org/10.1039/C8NJ01212A">https://doi.org/10.1039/C8NJ01212A</a>	YES
3.	A new carbazole-benzothiazole based chemodosimeter for chromogenic and fluorogenic detection of CN <sup>-</sup> . <i>Journal of Luminescence</i> , 201, pgs: 419 – 426.	Patra,L.; <b>Aich,K.</b> ;Gharami,S.;Mondal, T. K.	Chemistry	Journal of Luminescence	2018	0022-2313/1872-7883(online)	<a href="https://www.sciencedirect.com/journal/journal-of-luminescence">https://www.sciencedirect.com/journal/journal-of-luminescence</a>	DOI:10.1016/j.jlumin.2018.05.020	YES
4.	A new multi-analytefluorogenic sensor for efficient detection of Al <sup>3+</sup> and Zn <sup>2+</sup> ions based on ESIPT and CHEF features. <i>New Journal of Chemistry</i> , 42, pgs: 19076 – 19082.	Patra,L.;Das,S.;Gharami,S.; <b>Aich,K.</b> ;Mondal,T. K.	Chemistry	New Journal of Chemistry	2018	1144-0546/1369-9261 (online)	<a href="https://pubs.rsc.org/en/content/article/anding/2018/nj/c8nj03191f">https://pubs.rsc.org/en/content/article/anding/2018/nj/c8nj03191f</a>	<a href="https://doi.org/10.1039/C8NJ03191F">https://doi.org/10.1039/C8NJ03191F</a>	YES

5.	An ESIPT based chromogenic and fluorescent ratiometric probe for Zn <sup>2+</sup> with imaging in live cells and tissues. <i>New Journal of Chemistry</i> , 43, pgs: 1857 – 1863.	Gharami,S.; <b>Aich,K.</b> ;Sarkar,D.;Ghosh,P.;Murmu,N.;Mondal,T. K.	Chemistry	New Journal of Chemistry	2018	1144-0546/1369-9261 (online)	<a href="https://pubs.rsc.org/en/content/articleanding/2019/nj/c8nj04695f">https://pubs.rsc.org/en/content/articleanding/2019/nj/c8nj04695f</a>	<a href="https://doi.org/10.1039/C8NJ04695F">https://doi.org/10.1039/C8NJ04695F</a>	YES
6.	Size control synthesis and amperometric sensing activity of Palladium nanoparticles for Glucose detection, <i>Materials Today:Proceedings</i> , 5, pgs: 2049-2055.	A Mahajan, <b>S Banik</b> , S Roy Chowdhury, P.S. Roy, and S.K. Bhattacharya	Chemistry	Materials Today:Proceedings	2018	2214-7853	<a href="https://www.sciencedirect.com/journal/materials-today-proceedings">https://www.sciencedirect.com/journal/materials-today-proceedings</a>	<a href="https://doi.org/10.1016/j.matpr.2017.09.200">https://doi.org/10.1016/j.matpr.2017.09.200</a>	YES
7.	Adsorption of Dyes on nanocolloidal gold surfaces: The key towards understanding the mechanism of SERS, <i>Materials Today: Proceedings</i> , 5, pgs: 10042–10046.	<b>Dutta Roy, S.</b> , Chowdhury, J.	Physics	Materials Today:Proceedings	2018	2214-7853	<a href="https://doi.org/10.1016/j.matpr.2017.10.204">https://doi.org/10.1016/j.matpr.2017.10.204</a>	<a href="https://doi.org/10.1016/j.matpr.2017.10.204">https://doi.org/10.1016/j.matpr.2017.10.204</a>	YES
8.	Degradation of Methyl Parathion, a common pesticide and fluorescence quenching of Rhodamine B, a carcinogen using b-D glucan stabilized gold nanoparticles. <i>Journal of Saudi Chemical Society</i> ,22(8), pgs: 937-948.	Sutanuka Pattanayak, <b>Sharmila Chakraborty</b> , Suman Biswas, Dipankar Chattopadhyay , Mukut Chakraborty	Microbiology	Journal of Saudi Chemical Society	2018	1319-6103/2212-4640(online)	<a href="https://doi.org/10.1016/j.jscs.2018.02.004">https://doi.org/10.1016/j.jscs.2018.02.004</a>	<a href="https://doi.org/10.1016/j.jscs.2018.02.004">https://doi.org/10.1016/j.jscs.2018.02.004</a>	YES
9.	Therapeutic targeting of PFKFB3 with a novel glycolytic inhibitor PFK158promotes lipophagy and chemosensitivity in gynecologic cancers. 7.36), <i>Int J Cancer</i> . 1;144(1), pgs: 178-189.	<b>Mondal S</b> , Roy D, Sarkar Bhattacharya S, Jin L, Jung D, Zhang S, Kalogera E, Staub J, Wang Y, Xuyang W, Khurana A, Chien J, Telang S, Chesney J, Tapolsky G, Petras D, Shridhar V	Microbiology	Int J Cancer	2018	1097-0215/0020-7136	<a href="https://online.library.wiley.com/doi/full/10.1002/ijc.31868">https://online.library.wiley.com/doi/full/10.1002/ijc.31868</a>	<a href="https://onlinelibrary.wiley.com/doi/full/10.1002/ijc.31868">https://onlinelibrary.wiley.com/doi/full/10.1002/ijc.31868</a>	YES
10.	The Physics behind the Barrier to internal rotation of Acetyl Chloride molecule: A combined approach from DFT, Car Parrinello Molecular dynamics and time resolved wavelet transform theory. <i>ACS Omega</i> , 3,pgs: 6794 -6803.	<b>Bipan Dutta</b> , BiplabBhattacharjee, Joydeep Chowdhury.	Physics	ACS Omega	2018	2470-1343	<a href="https://pubs.acs.org/doi/10.1021/acsomega.8b00316">https://pubs.acs.org/doi/10.1021/acsomega.8b00316</a>	<a href="https://doi.org/10.1021/acsomega.8b00316">https://doi.org/10.1021/acsomega.8b00316</a>	YES
11.	Hydrogen bonded supramolecular architecture of a copper (II)-citrate	Sougata Sarkar, Dibakar Deb, Avijit Sarkar,	Physics	Indian J. of Chem.	2018	0019-5103	<a href="http://op.nisc.air.res.in/ind">http://op.nisc.air.res.in/ind</a>	DOI: 10.56042/ijca.v57i4	YES

	coordination building block: Synthesis and crystal structure with theoretical insight. <i>Indian J. of Chem.</i> 57A, pgs: 469-476.	Shouvik Chattopadhyay, <b>Bipan Dutta</b> , Soumen Khanra					<a href="http://ex.php/IJCA/article/view/20376/0">ex.php/IJCA/article/view/20376/0</a>	.20376	
12.	An (other) Quest for the Political: Ranjan Ghosh's Detechnification of Pedagogy Through Tagore. <i>Sanglap: Journal of Literary and Cultural Inquiry</i> , 5(1), pgs: 104-112.	<b>Samrat Sengupta</b>	English	Sanglap : Journal of Literary and Cultural Inquiry	2018	2349-8064	<a href="https://sanglap-journal.in/index.php/sanglap">https://sanglap-journal.in/index.php/sanglap</a>	<a href="https://sanglap-journal.in/index.php/sanglap/issue/view/9">https://sanglap-journal.in/index.php/sanglap/issue/view/9</a>	YES
13.	Solvent-Dependent Nanostructures Based on Active $\square$ -Aggregation Induced Emission Enhancement of New Carbazole Derivatives of Triphenylacrylonitrile. <i>Chemistry A European Journal</i> , 25(18), pgs: 4856 – 4863.	Maity, S.; <b>Aich, K.</b> ; Prodh an, C.; Chaudhuri, K.; Pra manik, A. K.; Das, S.; Ganguly, J.	Chemistry	Chemistry - A European Journal	2019	0947-6539/15 21-3765 (online)	<a href="https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/chem.201900312">https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/chem.201900312</a>	<a href="https://doi.org/10.1002/chem.201900312">https://doi.org/10.1002/chem.201900312</a>	YES
14.	Facile detection of organophosphorus nerve agent mimic (DCP) through a new quinolone based ratiometric switch. <i>New Journal of Chemistry</i> , 43(22), pgs: 8627 – 8633.	Gharami, S.; <b>Aich, K.</b> ; Das, S.; Patra, L.; Mondal, T. K.	Chemistry	New Journal of Chemistry	2019	1144-0546/13 69-9261 (online)	<a href="https://pubs.rsc.org/en/content/articlelanding/2019/nj/c9nj02218j">https://pubs.rsc.org/en/content/articlelanding/2019/nj/c9nj02218j</a>	<a href="https://doi.org/10.1039/C9NJ02218J">https://doi.org/10.1039/C9NJ02218J</a>	YES
15.	Simple fabrication of a carbaldehyde based fluorescent “turn-on” probe for the selective and sole detection of Pd <sup>2+</sup> : application as test strips. <i>New Journal of Chemistry</i> , 43, pgs: 16915 – 16920.	Manna, C.K.; Gharami, S.; <b>Aich, K.</b> ; Patra, L.; Mondal, T. K.	Chemistry	New Journal of Chemistry	2019	1144-0546/13 69-9261 (online)	<a href="https://pubs.rsc.org/en/content/articlelanding/2019/nj/c9nj04313f">https://pubs.rsc.org/en/content/articlelanding/2019/nj/c9nj04313f</a>	<a href="https://doi.org/10.1039/C9NJ04313F">https://doi.org/10.1039/C9NJ04313F</a>	YES
16.	Two New Quinoline-Benzothiazole Blended ‘Off-On’ Type Fluorescent Probes Exclusively Detect Cd <sup>2+</sup> . <i>Chemistry Select</i> , 4, pgs: 8068 – 8073.	<b>Aich, K.</b> ; Das, S.; Gharami, S.; Patra, L.; Mondal, T. K.	Chemistry	Chemistry Select	2019	2365-6549	<a href="https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/slct.201901582">https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/slct.201901582</a>	<a href="https://doi.org/10.1002/slct.201901582">https://doi.org/10.1002/slct.201901582</a>	YES
17.	Anodic Oxidation of Butan-1-ol on Reduced Graphene Oxide-Supported PdAg Nanoalloy for Fuel Cell Application., <i>ACS</i>	A. Mahajan, <b>S. Banik</b> , D. Majumdar, S. K. Bhattacharya	Chemistry	ACS Omega	2019	2470-1343	<a href="https://pubs.acs.org/journal/acsofd">https://pubs.acs.org/journal/acsofd</a>	<a href="https://pubs.acs.org/doi/10.1021/acso">https://pubs.acs.org/doi/10.1021/acso</a>	YES

	<i>Omega</i> , 4 (3),pgs: 4658-4670.							<a href="https://doi.org/10.1016/j.flatc.2019.10.011">mega.8b03561</a>	
18.	Temperature Control Synthesis of Platinum Nanoparticle-Decorated Reduced Graphene Oxide of different functionalities for anode-catalytic Oxidation of Methanol., <i>FlatChem</i> , 16, pgs: 100-111.	<b>S. Banik</b> , A. Mahajana, A. Ray, D. Majumdar, S. Das, S. K. Bhattacharya	Chemistry	FlatChem	2019	2452-2627	<a href="https://doi.org/10.1016/j.flatc.2019.10.011">https://doi.org/10.1016/j.flatc.2019.10.011</a>	<a href="https://doi.org/10.1016/j.flatc.2019.10.011">https://doi.org/10.1016/j.flatc.2019.10.011</a>	YES
19.	Size Control Synthesis of Pure Ni nanoparticles and Anodic-Oxidation of Butan-1-ol in Alkali., <i>Materials Chemistry and Physics</i> , 235, pgs: 121747.	<b>S. Banik</b> , A. Mahajan, S. K. Bhattacharya	Chemistry	Materials Chemistry and Physics	2019	1879-3312/0254-0584(Online)	<a href="https://doi.org/10.1016/j.matchemphys.2019.121747">https://doi.org/10.1016/j.matchemphys.2019.121747</a>	<a href="https://doi.org/10.1016/j.matchemphys.2019.121747">https://doi.org/10.1016/j.matchemphys.2019.121747</a>	YES
20.	Synthesis of a novel pyrene derived perimidine and exploration of its aggregation induced emission, aqueous copper ion sensing, effective antioxidant and BSA interaction properties., <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 377, pgs:236- 246.	N. Chakraborty, <b>S. Banik</b> , A. Chakraborty, S. K. Bhattacharya, S. Das	Chemistry	Journal of Photochemistry and Photobiology A: Chemistry	2019	1010-6030/1873-2666(online)	<a href="https://doi.org/10.1016/j.jphotochem.2019.03.014">https://doi.org/10.1016/j.jphotochem.2019.03.014</a>	<a href="https://doi.org/10.1016/j.jphotochem.2019.03.014">https://doi.org/10.1016/j.jphotochem.2019.03.014</a>	YES
21.	Existence of dimeric hydroxylamine O-sulfonic acid: Experimental observations aided by <i>ab initio</i> , DFT, Car-Parrinello and Born – Oppenheimer on the fly dynamics, <i>Chemical Physics Letters</i> , 732, pgs: 136645.	<b>Bipan Dutta</b> , Joydeep Chowdhury	Physics	Chemical Physics Letters	2019	2590-1419/1873-4448 (online)	<a href="https://doi.org/10.1016/j.cplett.2019.136645">https://doi.org/10.1016/j.cplett.2019.136645</a>	<a href="https://doi.org/10.1016/j.cplett.2019.136645">https://doi.org/10.1016/j.cplett.2019.136645</a>	YES
22.	Selective and sensitive detection of L-Cysteine via fluorometric assay using gold nanoparticles and Rhodamine B in aqueous medium, <i>Mat. Chem. Phys.</i> , 234, pgs:158-167.	Maiti, P, Singha, T., Chakraborty, U., <b>Dutta Roy, S.</b> , Karmakar, P., Dey, B., Hussain, S. A., Paul, S, Paul, P.K.	Physics	Materials Chemistry and Physics	2019	0254-0584/1879-3312 (online)	<a href="https://doi.org/10.1016/j.matchemphys.2019.06.001">https://doi.org/10.1016/j.matchemphys.2019.06.001</a>	<a href="https://doi.org/10.1016/j.matchemphys.2019.06.001">https://doi.org/10.1016/j.matchemphys.2019.06.001</a>	YES
23.	Study of interaction and its dynamics with reference to Spotted deer and Sambar populations at spatial scales, under the influence of resource and habitat heterogeneity: a case study with special reference to Kanha and Bandhavgarh National Park. <i>Environment and Ecology</i> , 37(1B), pgs: 373-386.	<b>Debashis, Roy</b> , and Mistry Kamonashish.	Zoology	Environment and Ecology	2019	0970-0420	<a href="https://www.environmentandecology.com/volume-37-2019">https://www.environmentandecology.com/volume-37-2019</a>	<a href="https://drive.google.com/file/d/1XSBEMUAnP9Ez_kFgrHTEOcea9f8nND8f/view">https://drive.google.com/file/d/1XSBEMUAnP9Ez_kFgrHTEOcea9f8nND8f/view</a>	YES
24.	Pulsatile flow and heat transfer of blood in	G. C. Shit, S. Maity, <b>M.</b>	Mathematics	Mathematics	2019	1872-	<a href="https://doi.org/10.1016/j.flatc.2019.10.011">https://doi.org/10.1016/j.flatc.2019.10.011</a>	<a href="https://doi.org/10.1016/j.flatc.2019.10.011">https://doi.org/10.1016/j.flatc.2019.10.011</a>	YES

	an overlapping vibrating atherosclerotic artery: A numerical study, <i>Mathematics and Computers in Simulation</i> , 166,pgs: 432-450.	<b>Roy</b> and J. C. Misra,		and Computers in Simulation		7166	<a href="https://doi.org/10.1016/j.matcom.2019.06.015">g/10.1016/j.matcom.2019.06.015</a>	<a href="https://doi.org/10.1016/j.matcom.2019.06.015">g/10.1016/j.matcom.2019.06.015</a>	
25.	Undecidable Spaces: Rethinking Caste and the Technologies of Abandonment in Manoranjan Byapari. <i>Sanglap:Journal of Literary and Cultural Inquiry</i> , 6(1), pgs:64-77.	<b>Samrat Sengupta</b>	English	Sanglap:Journal of Literary and Cultural Inquiry	2019	2349-8064	<a href="https://sanglap-journal.in/index.php/sanglap">https://sanglap-journal.in/index.php/sanglap</a>	<a href="https://sanglap-journal.in/index.php/sanglap/issue/view/12">https://sanglap-journal.in/index.php/sanglap/issue/view/12</a>	YES
26.	Introduction: Caste in/as Humanities: Unsettling the Politics of Suffering, <i>Sanglap:Journal of Literary and Cultural Inquiry</i> , 6(1), pgs:1-6.	Kalyan Kumar Das, <b>Samrat Sengupta</b>	English	Sanglap:Journal of Literary and Cultural Inquiry	2019	2349-8064	<a href="https://sanglap-journal.in/index.php/sanglap">https://sanglap-journal.in/index.php/sanglap</a>	<a href="https://sanglap-journal.in/index.php/sanglap/article/view/114">https://sanglap-journal.in/index.php/sanglap/article/view/114</a>	YES
27.	A fluorescent “ON–OFF–ON” switch for the selective and sequential detection of Hg <sup>2+</sup> and I <sup>-</sup> with applications in imaging using human AGS gastric cancer cells. <i>Dalton Transactions</i> , 49, pgs:187 – 195.	Gharami,S.; <b>Aich,K.</b> ;Ghosh,P.Patra,L.;Murmu,N.;Mondal, T. K.	Chemistry	Dalton Transactions	2020	1477-9226/1477-9234(online)	<a href="https://pubs.rsc.org/en/content/articlelanding/2020/dt/c9dt04245h">https://pubs.rsc.org/en/content/articlelanding/2020/dt/c9dt04245h</a>	<a href="https://doi.org/10.1039/C9DT04245H">https://doi.org/10.1039/C9DT04245H</a>	YES
28.	A simple coumarin based “fluorescent on” probe for the selective detection of Al <sup>3+</sup> along with its application in live cell imaging via AGS cell line. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 390, pgs: 112294.	Gharami,S.; <b>Aich,K.</b> ;Ghosh,P.;Patra,L.; Murmu, N.; Mondal, T. K.	Chemistry	Journal of Photochemistry and Photobiology A: Chemistry	2020	1010-6030/1873-2666(online)	<a href="https://doi.org/10.1016/j.jphotochem.2019.112294">https://doi.org/10.1016/j.jphotochem.2019.112294</a>	<a href="https://doi.org/10.1016/j.jphotochem.2019.112294">https://doi.org/10.1016/j.jphotochem.2019.112294</a>	YES
29.	Synthesis of $\alpha$ - $\beta$ Bi <sub>2</sub> O <sub>3</sub> heterojunction photocatalyst and evaluation of reaction mechanism for degradation of RhB dye under natural sunlight, <i>Ceramics International</i> , 46,pgs:7667-7680.	K. K. Bera, M.Chakraborty, M. Mondal, <b>S. Banik</b> , S. K. Bhattacharya	Chemistry	Ceramics International	2020	0272-8842/1873-3956(online)	<a href="https://doi.org/10.1016/j.ceramint.2019.11.269">https://doi.org/10.1016/j.ceramint.2019.11.269</a>	DOI:10.1016/j.ceramint.2019.11.269	YES
30.	Species Habitat relationships of spotted deer through Geo-Spatial analysis at Kanha National park: A cluster oriented study. <i>Eco. Env. &amp; Cons.</i> 26 (February Suppl. Issue), pgs: S183-S194.	<b>Mistry, Kamonashis</b> , and Debashis Roy.	Geography	Eco. Env. & Cons.	2020	0971–765X	<a href="http://www.envirotechjournals.com/article_abstract.php?aid=">http://www.envirotechjournals.com/article_abstract.php?aid=</a>	<a href="http://www.envirotechjournals.com/EEC/FebSupplIssue202">http://www.envirotechjournals.com/EEC/FebSupplIssue202</a>	YES

							<a href="#">10245&amp;iid=296&amp;jid=3</a>	<a href="#">0/EEC-27.pdf</a>	
31.	GEOSS: an intelligent methodology for identifying site suitability of air sample collection. <i>International Journal of Intelligent Systems Technologies and Applications</i> .19(5), pgs:421-443.	<b>Mistry, Kamonashish</b> , Biplab Biswas, Siwen Zhang, Tao Wu, Liang Zhou, Abdelfettah Benchrif, and Srimanta Gupta.	Geography	International Journal of Intelligent Systems Technologies and Applications	2020	1740-8865/1740-8873(online)	<a href="https://dl.acm.org/doi/10.1504/ijista.2020.111062">https://dl.acm.org/doi/10.1504/ijista.2020.111062</a>	<a href="https://doi.org/10.1504/ijista.2020.111062">https://doi.org/10.1504/ijista.2020.111062</a>	YES
32.	Technification of Knowledge and Knowledge as Technology: the University as the Verse to Come. <i>Rupkatha Journal on Interdisciplinary Studies in Humanities</i> , 12(5), pgs:1-6.	<b>Samrat Sengupta</b>	English	Rupkatha Journal on Interdisciplinary Studies in Humanities	2020	0975-2935	<a href="https://rupkatha.com/v12n5.php">https://rupkatha.com/v12n5.php</a>	DOI: 10.21659/rupkatha.v12n5.rioc1s2n1	YES
33.	Fabrication of a new fluorogenic probe for detection of phosgene in solution and vapor phase. <i>Sensors and Actuators B: Chemical</i> , 326, pgs: 128837.	Patra, L.; <b>Aich, K.</b> ; Gharami, S.; Mondal, T. K.	Chemistry	Sensors and Actuators B: Chemical	2021	0925-4005/1873-3077(online)	<a href="https://doi.org/10.1016/j.snb.2020.128837">https://doi.org/10.1016/j.snb.2020.128837</a>	<a href="https://doi.org/10.1016/j.snb.2020.128837">https://doi.org/10.1016/j.snb.2020.128837</a>	YES
34.	A Glimpse into Swami Vivekananda's Philosophy of Religion. <i>Shodh Sanchar</i> , Vol: 11, No: 41, pgs: 245-249.	<b>Bibek Manna</b>	Philosophy	Shodh Sanchar	2021	2229-3620	<a href="http://shodhsanchar.in/#">http://shodhsanchar.in/#</a>	NA	YES
35.	The Union of the Finite and The Infinite in the Philosophy of Rabindranath. <i>Shodh Sarita</i> , Vol: 8, No: 29, Pgs: 291-222.	<b>Bibek Manna</b>	Philosophy	Shodh Sarita	2021	2348-2397	<a href="http://seresearchfoundation.in/">http://seresearchfoundation.in/</a>	NA	YES
36.	Effect of montmorillonite clay on the fluorescence resonance energy transfer between two cationic dyes Acridine Orange and Rhodamine B in solution, transfer between two cationic dyes Acridine Orange and Rhodamine B. <i>Materials Today: Proceedings</i> , 46, pgs: 6275-6285.	Utsav Chakraborty, Pradip Maiti, Tanmoy Singha, <b>Ujjal Saren</b> , Alapan Pal, Pabitra Kumar Pau	Physics	Materials Today: Proceedings	2021	2214-7853	<a href="https://doi.org/10.1016/j.matpr.2020.05.047">https://doi.org/10.1016/j.matpr.2020.05.047</a>	<a href="https://doi.org/10.1016/j.matpr.2020.05.047">https://doi.org/10.1016/j.matpr.2020.05.047</a>	YES
37.	Interpretation of species habitat relationship and animal interaction through remote sensing with reference to spotted	<b>Roy, Debashis</b> , and Kamonashish Mistry.	Zoology	Eco. Env. & Cons.	2021	0971-765X	<a href="http://www.ejvirobiotechjournals.com">http://www.ejvirobiotechjournals.com</a>	<a href="http://www.ejvirobiotechjournals.com">http://www.ejvirobiotechjournals.com</a>	YES

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41.	Adsorption of 4-Mercapto Pyridine with Gold Nanoparticles Embedded in the Langmuir–Blodgett Film Matrix of Stearic Acid: SERS, XPS Studies Aided by Born–Oppenheimer on the Fly Dynamics, Time–Resolved Wavelet Transform Theory, and DFT, <i>ACS Omega</i> , 7(32) , pgs: 27818.	Somsubhra Saha, <b>Bipan Dutta</b> , Manash Ghosh , and Joydeep Chowdhury	Physics	ACS Omega	2022	2470-1343	<a href="https://pubs.acs.org/doi/10.1021/acsomega.1c07321">https://pubs.acs.org/doi/10.1021/acsomega.1c07321</a>	<a href="https://doi.org/10.1021/acsomega.1c07321">https://doi.org/10.1021/acsomega.1c07321</a>	YES
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43.	Nod factor-independent ‘crack-entry’ symbiosis in dalbergoid legume <i>Arachishypogaea</i> . <i>Environmental Microbiology</i> , 24(6), pgs. 2732-2746.	Guha, Sohini, Firoz Molla, <b>Monolina Sarkar</b> , Fernando Ibañez, Adriana Fabra, and Maitrayee Das Gupta.	Botany	Environmental Microbiology	2022	1462-2920	<a href="https://environmental-microbiology.onlinelibrary.wiley.com/doi/10.1111/1462-2920.15111">https://environmental-microbiology.onlinelibrary.wiley.com/doi/10.1111/1462-2920.15111</a>	<a href="https://doi.org/10.1111/1462-2920.15111">https://doi.org/10.1111/1462-2920.15111</a>	YES

							<a href="https://doi.org/10.1111/1462-2920.15888">0.1111/1462-2920.15888</a>	2920.15888	
44.	Interaction of hectorite clay with a phospholipid monolayer at air-saline interface in presence of a fluorescent dye. <i>Molecular Crystals And Liquid Crystals</i> , 738 (1), pgs: 31-49.	Tanmoy Singha, <b>Ujjal Saren</b> , Pradip Maiti, Utsav Chakraborty, Alapan Pal & Pabitra Kumar Paul	Physics	Molecular Crystals And Liquid Crystals	2022	1542-1406	<a href="https://www.tandfonline.com/doi/abs/10.1080/15421406.2021.2013590">https://www.tandfonline.com/doi/abs/10.1080/15421406.2021.2013590</a>	<a href="https://doi.org/10.1080/15421406.2021.2013590">https://doi.org/10.1080/15421406.2021.2013590</a>	YES
45.	Comparative and Selective Interaction of Amino Acid D-Cysteine with Colloidal Gold Nanoparticles in the Presence of a Fluorescent Probe in Aqueous Medium. <i>ACS Omega</i> , 7, pgs: 29013–29026.	Pradip Maiti, <b>Ujjal Saren</b> , Utsav Chakraborty, Tanmoy Singha, Sharmistha Paul, and Pabitra Kumar Paul	Physics	ACS Omega	2022	2470-1343	<a href="https://pubs.acs.org/journal/acsodf">https://pubs.acs.org/journal/acsodf</a>	<a href="https://doi.org/10.1021/acsomega.2c02725">https://doi.org/10.1021/acsomega.2c02725</a>	YES
46.	Geographical Appraisal of COVID-19 in West Bengal, India. <i>GeoJournal</i> , 87(4), pgs: 2641-2662.	Biswas, Biplab, Rabindranath Roy, Tanusri Roy, Sumanta Chowdhury, Asish Dhara, and <b>Kamonasish Mistry</b> .	Geography	Geo Journal	2022	0343-2521/1572-9893(online)	<a href="https://doi.org/10.1007/s10708-021-10388-4">https://doi.org/10.1007/s10708-021-10388-4</a>	<a href="https://doi.org/10.1007/s10708-021-10388-4">https://doi.org/10.1007/s10708-021-10388-4</a>	YES
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48.	Enhancement of Fluorescence Mediated by Silver Nanoparticles: Implications for Cell Imaging, <i>Langmuir</i> , 39(19), pgs: 6713–6729	Maiti, P., Sarkar, S., Singha, T., <b>Dutta Roy, S.</b> , Mahato, M, Karmakar, P., Paul, S., Paul, P. K.,	Physics	Langmuir	2023	0743-7463/1520-5827(online)	<a href="https://pubs.acs.org/doi/abs/10.1021/acs.langmuir.3c00204">https://pubs.acs.org/doi/abs/10.1021/acs.langmuir.3c00204</a>	DOI: 10.1021/acs.langmuir.3c00204	YES
49.	Light-responsive biodegradation of wastewater pollutants: New developments	<b>Monolina Sarkar</b>	Botany	Journal of Hazardous	2023	2772-4166	<a href="https://doi.org/10.1016/j.">https://doi.org/10.1016/j.</a>	<a href="https://doi.org/10.1016/j.">https://doi.org/10.1016/j.</a>	YES

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Principal  
Sammikani Mahavidyalaya  
E.M. Bypass, Baghatin  
Kolkata-700 094



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## Development of a new fluorescence ratiometric switch for endogenous hypochlorite detection in monocytes of diabetic subjects by dye release method

Sangita Das,<sup>a</sup> Krishnendu Aich,<sup>a</sup> Lakshman Patra,<sup>a</sup> Kakali Ghoshal,<sup>b</sup> Saswati Gharami,<sup>a</sup> Maitree Bhattacharyya<sup>b</sup> and Tapan Kumar Mondal<sup>a\*</sup>

<sup>a</sup> Department of Chemistry, Jadavpur University, Kolkata - 700032, India.

<sup>b</sup> Department of Biochemistry, University of Calcutta, Kolkata - 700019, India.

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### ABSTRACT

Increased oxidative stress in metabolic complications like type 2 diabetes, dyslipidemia and cardiovascular disorders exerts potential health hazards in many facets. Enhanced production of reactive oxygen species (ROS) due to increased oxidative stress promotes the damage of many biologically important macromolecules. Hypochlorous acid (HOCl), a microbicidal agent is also known to be an important ROS sub-species. An enhanced generation of endogenous HOCl due to diseased condition therefore can be detrimental to health. In present work, a new quinoline-diaminomaleonitrile based probe (HQMN) has been designed for the selective detection of hypochlorite. The probe in hand shows a selective ratiometric emission change towards OCl<sup>-</sup>. The probe behaves as a highly selective and sensitive tool for the detection of OCl<sup>-</sup> over other analytes with a fast response time (within 100 sec). Bioimaging study revealed that HQMN can detect endogenous OCl<sup>-</sup> in human monocytes and an increase in endogenous HOCl concentration has been witnessed in diabetic condition compared to healthy control. Thus HQMN can be used as an excellent fluorescent probe for dynamic tracking of hypochlorite in living biological cells especially to identify diabetic conditions.

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### Introduction

Hypochlorous acid (HOCl) acts as one of the most powerful microbicidal agent in the innate immune system,<sup>1</sup> which is slightly acidic and under physiological pH solutions it partially dissociates to give the hypochlorite ion (OCl<sup>-</sup>).<sup>2</sup> In living organisms, the endogenous hypochlorite is produced predominantly from the peroxidation of chloride ions catalyzed by the heme enzyme myeloperoxidase (MPO).<sup>3</sup> The produced hypochlorite is generally localized in activated macrophages, neutrophils and monocytes.<sup>4</sup> Hypochlorite plays crucial roles in human immune defence system by demolition of invading bacteria and pathogens.<sup>5</sup> Therefore, an enhanced endogenous HOCl can indicate a variety of diseases including type 2 diabetes mellitus,<sup>6</sup> dyslipidemia,<sup>6</sup> cardiovascular diseases,<sup>7</sup> neuron degeneration,<sup>8</sup> arthritis,<sup>9</sup> and cancer.<sup>10</sup> Type 2 diabetes mellitus, a metabolic complication is increasing rapidly across the globe causing death worldwide.<sup>11</sup> It is believed that type 2 diabetes increases endogenous HOCl by increased MPO as well as H<sub>2</sub>O<sub>2</sub> generation in both monocytes and neutrophils, two predominant white blood cells.<sup>10</sup> Therefore, significant effort has recently been focused on the fabrication of switches which can selectively detect HOCl in biological systems. A number of sensitive and selective analytical methods have been proposed for conducting such research.<sup>12</sup> Recently, a few fluorescence probes for OCl<sup>-</sup> have been reported based on the strong oxidation property of it.<sup>13</sup> Motivated by the above mentioned pioneering works, herein, we report the synthesis, photophysical characterization and cellular

imaging experiments of the quinoline-diaminomaleonitrile based chemodosimeter system (HQMN) which can selectively detects hypochlorite ion in a unique ratiometric manner. This is an in-situ approach where the target molecule (HQMN) reacted with the ROS (OCl<sup>-</sup>) to form the adduct (HQMN-OCl<sup>-</sup>), which on further hydrolysis liberated the dye (diaminomaleonitrile). The signalling approach was accomplished by a unique inorganic ion-induced dye releases method. We investigated that the probe in hand (HQMN) can detect not only hypochlorite selectively in presence of other ROS and guests but can also detect intracellular hypochlorite released in living blood cells. Bioimaging study also revealed that HQMN can effectively detect endogenous hypochlorite in living monocytes isolated from normoglycemic healthy control and type 2 diabetic subjects. We propose that novel probe HQMN is an excellent fluorescent marker to detect endogenous HOCl and can be used extensively in disease detection especially diabetes. These results suggest that the probe (HQMN) is an efficient one which can distinguish diabetic cells from normal cells by hypochlorite-induced dye releases method.

### Results and discussion

#### Synthesis of the probe (HQMN)

The synthetic procedure for the synthesis of the probe (HQMN) is outlined in Scheme 1. 8-methoxyquinoline-2-carbaldehyde (HQA) is prepared by following literature procedure.<sup>14</sup> Condensation of HQA with 1,2-diaminomaleonitrile affords the probe (HQMN) as yellow crystalline solid. Detailed

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ARTICLE

## Detection and discrimination of Zn<sup>2+</sup> and Hg<sup>2+</sup> using a single molecular fluorescent probe

Saswati Gharami, Krishnendu Aich, Lakshman Patra and Tapan K. Mondal\*

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A new fluorescent probe (SAPH) has been introduced which shows specific sensing towards Zn<sup>2+</sup> and Hg<sup>2+</sup> in two different wavelength maxima at physiological pH. The probe shows a brilliant ratiometric red shift in emission spectra upon addition of Zn<sup>2+</sup> at 678 nm while Hg<sup>2+</sup> shows a turn-on ratiometric emission enhancement with a red shift at 647 nm. Job's plot confirms the 1:1 complexation for both Zn<sup>2+</sup> and Hg<sup>2+</sup>. Binding constants have been calculated using Benesi-Hildebrand equation and found to be 3.03×10<sup>5</sup> M<sup>-1</sup> and 6.05×10<sup>4</sup> M<sup>-1</sup> respectively for SAPH-Zn<sup>2+</sup> and SAPH-Hg<sup>2+</sup>. DFT and TDDFT studies are conducted with the probe to establish a similarity between theoretical and experimental outcomes.

### Introduction

In recent days, the area of highly luminescent chemosensors has been of great interest owing to their various applications in photoelectronic diodes, biotechnology and memory system.<sup>1-5</sup> A large amount of fluorescent chemosensors which have been reported till are based on organic moieties as they are simple-to-use, cost effective and easy to handle.<sup>6-9</sup> The development of bifunctional fluorescent probes which selectively discriminates more than two metal ions or anions have been a very interesting area in the fluorescence studies recently.<sup>10-16</sup> Environmental contamination by heavy toxic metals is becoming a great threat in recent days due to the accumulation of these pollutants in water and foods which have led to various dangerous diseases in living beings.<sup>17</sup> Among the heavy metals, mercury is a highly toxic metal whose presence in environment causes great threat not only for the ecological system but also for the human health.<sup>18</sup> Mercury can be widely spread into the environment via various sources such as gold production, coal plants, thermometers, barometers, mercury lamps etc.<sup>19</sup> Even exposure to very small concentration of mercury can cause strong damage to the central nervous system.<sup>20</sup> Thus the long term accumulation of mercury in the human body can lead to various cognitive and motor disorders along with pulmonary edema, cyanosis, nephritic syndrome and Minamata disease.<sup>21</sup> So although many fluorescent probes are reported for the detection of Hg<sup>2+</sup> in literature,<sup>22</sup> there is still an urgent need of developing a sensitive and appropriate Hg detection method. Zinc being the second most abundant transition metal after

iron has various important roles in catalytic activity, neurological activity, gene transcription and cellular transport.<sup>23</sup> But unregulated zinc level in human body may lead to several dangerous diseases such as β-thalassemia, Friedreich's ataxia, and neurodegenerative diseases including Alzheimer's disease, Parkinson's disease and epilepsy.<sup>24-26</sup> The disorder of zinc level also leads to the probability of prostate cancer.<sup>27</sup> Furthermore detection of zinc is also very much needed for the sake of environment as it is a harmful metal pollutant too.<sup>28</sup> Therefore it is highly desirable and demandable to develop a powerful and sensitive analytical tool for the detection of Hg<sup>2+</sup> and Zn<sup>2+</sup> in environmental sample. There are many successful fluorescent probes reported to date which can selectively detects these two metal ions individually.<sup>29,30</sup> However, to detect one of these metals individually, there is some interference observed from the other one.<sup>31</sup> Therefore, it remains a challengeable task to design a single molecular probe that not only can recognize but also can discriminate these two metal ions belonging to the same group.

In this paper, we have investigated a simple idea for Zn<sup>2+</sup> and Hg<sup>2+</sup> specific probe design. So we have introduced a new fluorescent switch which exhibits fluorescence "turn-on" response towards Zn<sup>2+</sup> and Hg<sup>2+</sup> specifically in two different wavelength regions thereby discriminating the duo via one probe.

### Experimental

#### General Procedures

All reagents and solvents used in this synthesis were purchased from Aldrich. All other organic chemicals and inorganic salts were available from commercial sources and used without further purification. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on Bruker 300 MHz instrument. For NMR spectra, CDCl<sub>3</sub> and DMSO-d<sub>6</sub> were used as solvents (mentioned

Department of Chemistry, Jadavpur University, Kolkata-700032, India. E-mail: tapank.mondal@jadavpuruniversity.in  
†Electronic Supplementary Information (ESI) available: [NMR and MS of all new compounds, Limit of detection determination, Quantum yield calculation etc.]. See DOI: 10.1039/x0xx00000x

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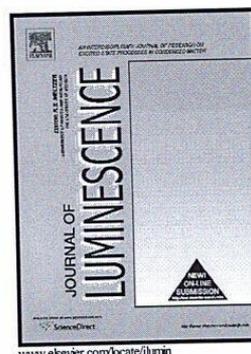
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Principal  
Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

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## Author's Accepted Manuscript

A new carbazole-benzothiazole based chemodosimeter for chromogenic and fluorogenic detection of  $\text{CN}^-$

Lakshman Patra, Krishnendu Aich, Saswati Gharami, Tapan Kumar Mondal



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## A new carbazole-benzothiazole based chemodosimeter for chromogenic and fluorogenic detection of $\text{CN}^-$

Lakshman Patra, Krishnendu Aich, Saswati Gharami and Tapan Kumar Mondal\*

Department of Chemistry, Jadavpur University, Kolkata-700032, India.

Corresponding author: Ph: 91-033-24572970; Email: tapank.mondal@jadavpuruniversity.in

### Abstract

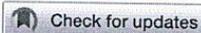
A hybrid carbazole-benzothiazole based chemodosimeter (CB) has been synthesized for the colorimetric and fluorogenic detection of cyanide ion ( $\text{CN}^-$ ). Intra-molecular charge transfer (ICT) played important role for the detection of  $\text{CN}^-$  in DMSO-water (4/1, v/v, pH=7.2) solution. Upon treatment of  $\text{CN}^-$  to the probe solution, results bleaching of the original yellow color of the probe with a large blue shift in absorption spectra. A large enhancement of the fluorescence intensity with a slight red shift is observed after addition of  $\text{CN}^-$  to the probe (CB). Here, the nucleophilic addition of  $\text{CN}^-$  inhibits the intra-molecular charge transfers (ICT) process responsible for the large enhancement of emission. The chemical reaction involved behind the sensing of  $\text{CN}^-$  has been confirmed through  $^1\text{H}$  NMR and mass spectroscopic studies. The density function theory (DFT) and time-dependent density function theory (TDDFT) has also been conducted to support the experimental findings.

### Graphical Abstract:

The synthesized carbazole-benzothiazole based chemodosimeter (CB) is selectively used for the colorimetric and fluorogenic detection of cyanide ion ( $\text{CN}^-$ ). Both intra-molecular charge

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*Patra*  
Principal  
Sammahi Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

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## A new multi-analyte fluorogenic sensor for efficient detection of Al<sup>3+</sup> and Zn<sup>2+</sup> ions based on ESIPT and CHEF features†

Lakshman Patra, Sangita Das, Saswati Gharami, Krishnendu Aich and Tapan Kumar Mondal\*

The fluorogenic chemosensor 3-(((2-hydroxy-4-methylphenyl)imino)methyl)-[1,1'-biphenyl]-4-ol (H<sub>2</sub>L) efficiently detects Zn<sup>2+</sup> and Al<sup>3+</sup> ions and subsequently fluoride ion in methanol–water (4/1, v/v, pH = 7.2) solution. The probe itself is non-emissive but upon treatment with Al<sup>3+</sup> and Zn<sup>2+</sup>, it exhibits high fluorescence emission at two different wavelengths of 546 nm and 529 nm, respectively. Both excited-state intramolecular proton transfer (ESIPT) and chelation enhanced fluorescence (CHEF) processes play important roles in the enhancement of fluorescence intensity. Chelation of Zn<sup>2+</sup> and Al<sup>3+</sup> with the probe (H<sub>2</sub>L) inhibits C=N isomerization and ESIPT which consequently enhances the emission intensity. The emission intensity of H<sub>2</sub>L–Al<sup>3+</sup> is selectively quenched upon titration with F<sup>−</sup> anions. The structure of the probe is confirmed by the single crystal X-ray diffraction method. The electronic structure and sensing mechanism of the probe (H<sub>2</sub>L) are supported by density functional theory (DFT) and time-dependent density functional theory (TDDFT).

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### Introduction

There are many versatile applications of organic probes in different fields such as chemistry, biology and the environment for the selective detection of chemical and biological species.<sup>1,2</sup> The detection mechanism of most chemosensors is based on metal–ligand coordination,<sup>3–5</sup> electrostatic interactions,<sup>6–8</sup> hydrogen bonding,<sup>9–11</sup> van der Waals forces<sup>12</sup> and hydrophobic interactions.<sup>13–15</sup> Among them, the metal–ligand chelation enhanced fluorescence (CHEF) approach is most exciting as visualization and imaging both are possible due to the fluorescence turning on after interaction with the guest analyte. Chemosensors with different responses towards different analytes are highly desirable. But it is challenging to develop such a probe. So there is great research interest in this field in recent times.

Aluminum is the third most abundant element in the biosphere, and nearly 8% of the total mineral component is aluminum. It is widely used in our daily life such as for food packaging, drinking water supplies, cookware, deodorant, bleached flour, antiperspirants, antacids and the manufacturing of cars and computers.<sup>16–18</sup> Although it is extensively used in our modern life, it

is harmful to both our environment and biological system. Al(III) leaches from soil during acid rain, deadly for growing plants.<sup>19–22</sup> Abnormal concentrations of aluminum in our body cause various dangerous diseases such as Alzheimer's, Parkinson's disease, bone softening, impaired lung function, fibrosis, chronic renal failure *etc.*<sup>23–26</sup> According to the WHO, regulation of the maximum Al(III) present in drinking water should be up to 7.42 μM and daily intake should be less than 3–10 mg.<sup>27–29</sup> Therefore, due to environmental and health concerns, it is necessary to develop a chemosensor for the detection of Al(III).

On the other hand, zinc is the second most abundant element in the human body.<sup>30</sup> It plays an important role in gene transcription, cellular metabolism, immunological functions and signaling processes in the brain.<sup>31–33</sup> Although it is an essential trace element in the human body, excessive amounts of this metal can cause several neurological disorders such as Alzheimer's and Parkinson's diseases.<sup>34,35</sup> Up to 8–11 mg per day of Zn(II) intake is tolerable for maintaining good health.<sup>36</sup> In the presence of higher concentrations of zinc in the human body, other essential trace elements such as iron, copper *etc.* cannot work properly.<sup>37</sup>

Fluoride sensing is also one of the most attractive fields of research nowadays as it has immense potential in biology and chemistry.<sup>38,39</sup> Excessive amounts of fluoride can cause several diseases in our body such as urolithiasis, osteoporosis, stomach ulcers or even cancer.<sup>40–43</sup> There are very few chemosensors which can detect both Al(III) and Zn(II) and sequentially fluoride anions as it

Department of Chemistry, Jadavpur University, Kolkata 700032, India.

E-mail: tapank.mondal@jadavpuruniversity.in

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Sammisahi Mahavidyalaya  
E.M. Bypass, Baghejatin  
Kolkata-700094

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## An ESIPT based chromogenic and fluorescent ratiometric probe for Zn<sup>2+</sup> with imaging in live cells and tissues†

 Saswati Gharami,<sup>a</sup> Krishnendu Aich,<sup>b</sup> Deblina Sarkar,<sup>‡</sup> Paramita Ghosh,<sup>b</sup>  
 Nabendu Murmu<sup>\*b</sup> and Tapan Kumar Mondal<sup>†\*</sup>

A new ESIPT based fluorescent probe has been introduced for selective detection of Zn<sup>2+</sup> in human breast cancer cells. The designed probe exhibits a prominent ratiometric fluorescence change along with a sharp blue shift of ~71 nm which can be attributed to the hampering of the ESIPT process. The probe is efficient enough to detect Zn<sup>2+</sup> solely in the presence of other biologically relevant cations with a limit of detection value of 1.6 × 10<sup>-7</sup> M. The experimentally observed changes in the structure and absorption properties of the probe after complete addition of Zn<sup>2+</sup> were further studied by density functional theory (DFT) and time dependent density functional theory (TDDFT) calculations. Moreover, the dip-stick experiment with this probe displays both absorption and fluorescence color changes after exposure to Zn<sup>2+</sup> which also turns out to be a potential application for the probe. Live cell imaging studies have been carried out using human breast cancer cells (MCF-7) and tissues.

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### Introduction

Rapid and selective recognition of ions in aqueous media has become a vital part of research currently. This is very much needed in order to protect the environment, to monitor all the biological processes and also for identification of several diseases. Among an array of detection methods, the fluorescence based sensing technique has been proved to be of immense importance due to its simplicity, sensitivity, high degree of specificity, low detection limit, cost-effectiveness and short response time.<sup>1</sup> To date several fluorescent chemosensors have been developed for detecting many metal cations.<sup>2</sup> Zinc is the second most abundant transition metal in the human body after iron and it is also an essential trace mineral comprising more than 250 metalloenzymes.<sup>3</sup> There are several different biological functions where dependency on zinc is very much desired such as our immune system functions, DNA synthesis, neural signal transmission, apoptosis regulation, mammalian reproduction, cellular transport, metabolism and overall growth of the human body.<sup>4</sup> Zinc actively participates in various biological processes such

as oxygen transport,<sup>5</sup> gene expression<sup>6</sup> and cellular metabolism.<sup>7</sup> But the discrepancy of zinc ion concentration in the human body may lead to several life alarming diseases such as Alzheimer's disease,<sup>8</sup> epilepsy,<sup>9</sup> ischemic stroke,<sup>10</sup> prostate cancer<sup>11</sup> and Parkinson's disease.<sup>12</sup> Zinc is also a harmful environmental pollutant.<sup>13</sup> Hence there is an urgent need to develop chemosensors for the efficient detection of zinc, both 'in vivo' as well as 'in vitro'. The difficulty in sensing zinc distinctly in some intricate biological systems is attributed to the fact that zinc ions are silent to some common analytical techniques like Mossbauer, NMR and electron paramagnetic resonance (EPR) compared to other transition metal ions. Thus the detection of zinc with the help of fluorescent chemosensors is now a widely popular area of research. Due to the huge demand, several sensing devices involving different Schiff's bases, polythiacrown ethers, *etc.* have been developed in the past few years,<sup>14</sup> although most of them have the drawback of inadequate selectivity towards Zn<sup>2+</sup> due to special interference from Cd<sup>2+</sup> ions.<sup>15</sup> To date, many zinc sensors have been reported,<sup>16</sup> and a few of them show ratiometric fluorescence response. Despite of those nicely designed probes, there is still a great need to fabricate new ratiometric fluorescent probes which can selectively detect Zn<sup>2+</sup> in environmental as well as biological samples.

Herein a new fluorescent chemosensor (HBS) has been introduced which selectively binds to Zn<sup>2+</sup> over other metal cations with high sensitivity. The probe shows a profound ratiometric change in the emission spectra upon addition of Zn<sup>2+</sup>. The probe, HBS, can also detect Zn<sup>2+</sup> in live human breast cancer cells and

<sup>a</sup> Department of Chemistry, Jadavpur University, Kolkata-70003, India.  
E-mail: tapank.mondal@jadavpuruniversity.in

<sup>b</sup> Department of Signal Transduction and Biogenic Amines (STBA),  
Chittaranjan National Cancer Institute, Kolkata-700026, India

† Electronic supplementary information (ESI) available. See DOI: 10.1039/c8nj04695f

‡ Present address: Department of Chemistry, Bagnan College, Howrah, WB 711303, India.

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## Size control synthesis and amperometric sensing activity of Palladium nanoparticles for Glucose detection

A Mahajan, S Banik, S Roy Chowdhury, P. S.Roy and S. K.Bhattacharya\*

*Jadavpur University, Kolkata-700032, India*

\* Corresponding author. Tel.: +919831699643; fax: +913324146584.  
E-mail address: [skbhatt7@yahoo.co.in](mailto:skbhatt7@yahoo.co.in)

### Abstract

Size controlled synthesis of palladium nanoparticles of varying average diameter ranging from 8.1 to 21.3 nm, was executed by controlling the time of reflux of the facile reduction of PdCl<sub>2</sub> in a single pot using citric acid as reducing agent in presence of the steric stabilizer poly vinyl alcohol in water. The as synthesized nanomaterials were analysed by different microscopic techniques and utilized for the construction of a few anode-catalysts for biosensing of glucose. The catalytic activity of the anodes was characterized by cyclic voltammetry and chronoamperometry in different glucose solutions of varying concentration in 0.1M aqueous alkali. The maximum sensitivity is 66.2.µA cm<sup>-2</sup> mM<sup>-1</sup> found at the potential of 0.1V with respect to HgO/Hg electrode, for the particles having optimum crystallite-diameter of 12nm obtained from the solution having reflux time of 1.5 hour. The lowest limit (8.33 µM) and long linear range of detection (8.33 to 166 µM) are also important parameters of the best sensor studied. The results seem to help a better understanding and improvement of Palladium-based amperometric glucose sensor.

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*Keywords:* Palladium nanoparticles, amperometric glucose biosensor

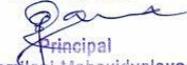
### 1. Introduction

In the last decade, nanoscience and technology have offered exciting prospects in biosensors by introducing novel nanomaterials, which include, but are not limited to, nanotubes, quantum dots, nanofibers, nanorods, and nano plates etc. [1, 2]. Possessing a number of remarkable advantages over conventional materials, nanomaterials are suitable for integration into novel mini, micro and nanodevices. These features use ultra-small sizes, large surface to volume

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IC-FNM 2016

## Adsorption of Dyes on nanocolloidal gold surfaces: The key towards understanding the mechanism of SERS.

Sannak Dutta Roy<sup>a</sup>, Joydeep Chowdhury<sup>a\*</sup>

<sup>a</sup>Department of Physics, Jadavpur University, 188, Raja S.C. Mallick Road, Jadavpur, Kolkata 700032, India

### Abstract

The adsorptive parameters of biologically significant Methylene Blue (MB) and Malachite Green (MG) dye molecules adsorbed on gold nanocolloidal particles of varied sizes have been reported with the aid of fluorescence spectroscopy study. Fluorescence spectroscopic studies have been further applied to estimate the concentration of probe molecules actually adsorbed on gold nanocolloidal particles surface. The effects of graphene oxide (GO) on the adsorptive parameters of MG molecule are also been estimated.

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**Keywords:** Fluorescence Spectroscopy; Absorption Spectroscopy; Adsorptive parameters; Gold nanocolloids.

### 1. Introduction

Surface Enhanced Raman Scattering (SERS) is characterized by large enhancement of Raman signals from molecules at trace concentrations down to single molecule detection limit [1]. It is a highly efficient spectroscopic technique to understand the adsorptive behaviours of probe molecules with the nanostructured surfaces [2]. The exact mechanism behind the phenomenon is still unknown, albeit, it is generally believed that a long range electromagnetic (EM) and a short range charge transfer (CT) mechanisms are simultaneously operative [3, 4]. Since, the accidental discovery of SERS, gold and silver nanocolloids are established as proven SERS active substrates for recording the vibrational signatures of wide range of organic molecules at ultrasensitive concentrations. The

\*Corresponding author. Tel.: 033-24138917;

E-mail address: [joydeepc@phys.jdvu.ac.in](mailto:joydeepc@phys.jdvu.ac.in) / [joydeep72\\_c@rediffmail.com](mailto:joydeep72_c@rediffmail.com)

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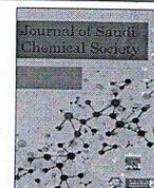
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E.M. Bypass, Baghajatin  
Kolkata-700094



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## ORIGINAL ARTICLE

# Degradation of Methyl Parathion, a common pesticide and fluorescence quenching of Rhodamine B, a carcinogen using $\beta$ -D glucan stabilized gold nanoparticles

Sutanuka Pattanayak<sup>a</sup>, Sharmila Chakraborty<sup>b</sup>, Suman Biswas<sup>a</sup>,  
Dipankar Chattopadhyay<sup>c</sup>, Mukut Chakraborty<sup>a,\*</sup>

<sup>a</sup> Department of Chemistry, West Bengal State University, Barasat, Kolkata 700126, West Bengal, India

<sup>b</sup> Department of Microbiology, Sammilani Mahavidyalaya, Baghajatin, E.M. Bypass, Santoshpur, Kolkata 700094, West Bengal, India

<sup>c</sup> Department of Polymer Science & Technology, University of Calcutta, 92, A.P.C. Road, Kolkata 700009, West Bengal, India

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## KEYWORDS

$\beta$ -D-Glucan;  
Gold nanoparticles;  
Green synthesis;  
Methyl Parathion;  
Fluorescence quencher

**Abstract** Natural carbohydrate polymer  $\beta$ -D-glucan extracted from *Tricholoma crassum* (Berk.) Sacc. predominantly linked by  $\beta$ -glycosidic bonds have been used to synthesize gold nanoparticles (Au NPs). As glucan is water soluble, the Au NPs are prepared in water medium, a green solvent. The morphology and characterization of the synthesized Au NPs have been confirmed by various techniques, like TEM, EDX, XRD, UV-Vis and FT-IR spectroscopic studies. The obtained Au NPs exhibits chemosensing property against Methyl Parathion, a group of highly toxic organophosphorous pesticide, extensively used as an agricultural chemical. Degradation of parathion using Au NPs lead to water-soluble products thereby reducing the toxicity of Methyl Parathion by disrupting the thiophosphate-ester linkage. The synthesized Au NPs also act as a good fluorescence quencher of Rhodamine B, a common fluorophore and carcinogenic compound, obeying Stern-Volmer equations. The  $\beta$ -D-glucan capped Au NPs are safe having possible medicinal usage.

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## 1. Introduction

Physico-chemical properties of metal nanoparticles have been extensively studied, leading to their use in different fields like catalysis, optics, electronics, and biotechnology [1–5]. Noble metal nanoparticles like Silver and Gold have proved their versatility in application areas such as catalysis [6,7], biological sensing and imaging [8], optics [9], chemical sensor [10],

\* Corresponding author.

E-mail address: mukutchem@yahoo.co.in (M. Chakraborty).

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E.M. Bypass, Baghajatin  
Kolkata-700094



**Therapeutic targeting of PFKFB3 with a novel glycolytic inhibitor PFK158 promotes lipophagy and chemosensitivity in gynecologic cancers**

Susmita Mondal<sup>1,7\*</sup>, Debarshi Roy<sup>1\*</sup>, Sayantani Sarkar Bhattacharya<sup>1</sup>, Ling Jin<sup>1</sup>, Deokbeom Jung<sup>1</sup>, Song Zhang<sup>2</sup>, Eleftheria Kalogera<sup>3</sup>, Julie Staub<sup>1</sup>, Yaxian Wang<sup>1</sup>, Wen Xuyang<sup>1</sup>, Ashwani Khurana<sup>1</sup>, Jeremy Chien<sup>4</sup>, Sucheta Telang<sup>5</sup>, Jason Chesney<sup>5</sup>, Gilles Tapolsky<sup>6</sup>, Dzeja Petras<sup>2</sup>, and Viji Shridhar<sup>1#</sup>

**Affiliations:**

<sup>1</sup>Department of Experimental Pathology, Mayo Clinic, Rochester, MN, USA.

<sup>2</sup>Division of Cardiovascular disease, Department of Medicine, Mayo Clinic, Rochester, MN, USA

<sup>3</sup>Division of Gynecologic Surgery, Department of Obstetrics and Gynecology, Mayo Clinic, Rochester, MN, USA

<sup>4</sup>Division of Molecular Medicine, University of New Mexico School of Medicine, Albuquerque, NM, USA

<sup>5</sup>Department of Medicine, University of Louisville, Louisville, KY, 40202, USA

<sup>6</sup>Advanced Cancer Therapeutics, Louisville, KY, 40202, USA

<sup>7</sup>Department of Microbiology, Sammilani Mahavidyalaya, Kolkata, India

\* These authors have contributed equally to this work

**Key Words:** Ovarian and Cervical Cancer, Chemoresistance, PFKFB3, lipid droplet, lipophagy

**Abbreviation:**

OC: Ovarian Cancer; F2,6BP: Fructose 2,6bis-phosphate; PFKFB3:6-phosphofructo-2-kinase/fructose-2,6-biphosphatase 3; FASN: fatty acid synthase; ACC:Acetyl Co-A carboxylase; ACLY: ATP citrate lyase; TAG: Triacylglycerol; CE: Cholesterol esters; LD: Lipid droplet; LCFA: Long chain fatty acids; CI: Combination index; DRI: Dose reduction index; CBPT: Carboplatin; PTX:Paclitaxel; IHC: Immunohistochemistry; IFC: Immunofluorescence; FTE: fallopian tube epithelial BafA: Bafilomycin A; AA: arachidonic acid; TG: triglycerides

**#Corresponding Author:**

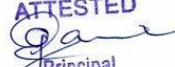
**Dr. Viji Shridhar**

Department of Experimental Pathology,  
Mayo Clinic College of Medicine,  
Rochester, MN 55905, USA

Email: [shridhar.vijayalakshmi@mayo.edu](mailto:shridhar.vijayalakshmi@mayo.edu)

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# Physics behind the Barrier to Internal Rotation of an Acetyl Chloride Molecule: A Combined Approach from Density Functional Theory, Car–Parrinello Molecular Dynamics, and Time-Resolved Wavelet Transform Theory

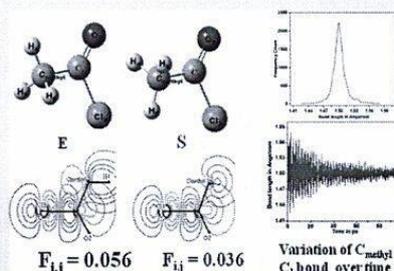
Bipan Dutta,<sup>†</sup> Biplab Bhattacharjee,<sup>‡</sup> and Joydeep Chowdhury<sup>\*§</sup>

<sup>†</sup>Department of Physics, Sammilani Mahavidyalaya, E. M. Bypass, Baghajatin Station, Kolkata 700094, India

<sup>‡</sup>Department of Chemistry and <sup>§</sup>Department of Physics, Jadavpur University, 88, Raja S. C. Mallick Road, Kolkata 700032, India

**S** Supporting Information

**ABSTRACT:** The physics behind the barriers to internal rotation of acetyl chloride (AC) molecule has been reported. The AC molecule closely resembles the molecular structure of acetaldehyde; the only subtle difference is the presence of a heavy chlorine atom in place of the hydrogen atom of the aldehyde group for the latter. This paper aims to study the effect of substitution of the heavy chlorine atom on the barrier energetics of the AC molecule. The reason behind the barrier for the AC molecule has been estimated for the first time from the unified approach using barrier energetics, natural bond orbital, nuclear virial, and relaxation analyses using density functional theory, Car–Parrinello molecular dynamics, and wavelet transform theory. Complete analyses reveal the concomitant relaxations of both the in-plane  $C_{\text{methyl}}-C_1$  and  $C_{\text{methyl}}-H_4$  bonds toward understanding the origin of the barrier due to internal rotation for the AC molecule. The large negative value of “ $V_6$ ” further suggests that both the abovementioned degrees of freedom are coupled with the  $-CH_3$  torsional vibration of the molecule. The coupling matrix ( $H_{12}$ ) element has also been estimated. Time-resolved band stretching frequencies of  $C_{\text{methyl}}-C_1$  and  $C_1-Cl_3$  bonds of the AC molecule, as obtained from wavelet transformation analysis, primarily preclude the possibility of coupling between the  $C_1-Cl_3$  bond and the torsional motion associated with the methyl group of the molecule.



## 1. INTRODUCTION

Molecular conformations play important roles in the world of macromolecules, whose structure–function relationship contributes significantly toward understanding the basic physics and chemistry behind the functioning of complex biological systems.<sup>1</sup> A molecule, in principle, can undergo conformational changes by internal rotation, ideally about the concerned single bond/bonds. The text book example of such internal rotation is observed in ethane, as it takes the stereoisomeric eclipsed and staggered conformations with the change in the specific dihedral angle. However, the real existence of this type of stereoisomeric conformers apparently seems to depend explicitly on the torsional angle  $\tau$ .<sup>2</sup> The barrier energy or height that separates two distinct conformations is fundamentally the effect of hindered rotation, stemming toward the concept of barrier potential. Interestingly, the quantum mechanical nature of hindered rotation was first identified by Nielsen in 1932.<sup>3</sup> The theoretical results from his group provide the initial plunge behind the phenomenal paper by Pitzer<sup>4</sup> on the internal rotation of the ethane molecule. Since then, the estimations of barrier heights have been extended to other molecules involving three- or even 6-fold barriers.<sup>5</sup> The results were primarily collected with the aid of microwave

spectroscopy from the splitting of rotational transitions into doublet, triplet, and quadruplet structures because of the internal rotation of the rotor group. Other experimental approaches to find barrier heights of conformeric molecules are from Raman and far-infrared spectroscopic investigations. For both these techniques, the torsional fundamental and overtone vibrational signatures provide the means of such estimations.<sup>6</sup> Moreover, fluorescence, supersonic jet-cooled, and the analyses of hot bands from UV–vis electronic spectroscopy also provide wealth of information toward the estimations of barriers heights.<sup>7</sup> Intriguingly, in the late fifties and early sixties of the twentieth century, Wilson et al. implicitly linked the origin of barrier heights with the electronic structures of molecules.<sup>8</sup> Understanding the origin of rotational barriers from the electronic structures of molecules was further facilitated by the advancement of quantum chemical calculations.<sup>9</sup> However, increasing availabilities of faster computations allow us to undergo in depth quantum mechanical studies to elucidate the unexplored physics behind the origin of

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## Hydrogen bonded supramolecular architecture of a copper(II)-citrate coordination building block: Synthesis and crystal structure with theoretical insight

Sougata Sarkar<sup>a,\*</sup>, Dibakar Deb<sup>b,\*</sup>, Avijit Sarkar<sup>c,\*</sup>,  
Shouvik Chattopadhyay<sup>d,\*</sup>, Bipan Dutta<sup>e</sup> & Soumen Khanra<sup>a</sup>

<sup>a</sup>Department of Chemistry, Ramakrishna Mission Vivekananda Centenary College,  
Rahara, Kolkata 700 118, India

Email: sougata.sarkar81@gmail.com

<sup>b</sup>Department of Chemistry, Techno India, Agartala 799 004, India

Email: debdibakar@gmail.com

<sup>c</sup>Department of Chemistry, Bhairab Ganguly College, Kolkata 700 056, India

Email: rite2avijit@gmail.com

<sup>d</sup>Department of Chemistry (Inorganic Section) Jadavpur University, Kolkata 700 032, India

Email: shouvik.chem@gmail.com

<sup>e</sup>Department of Physics, Sammilani Mahavidyalaya, Kolkata 700 094, India

Email: bipan.dutta@yahoo.com

A tricarboxylate supported binuclear metal organic hybrid of Cu(II), [Cu<sub>2</sub>(μ-cit)(phen)<sub>2</sub>]·9H<sub>2</sub>O (1) has been synthesized using the well known pyridyl based *N,N'* linker, 1,10-phenanthroline and structurally characterized. The use of the flexible hydroxyl tricarboxylate citrate, in designing such a framework has created a marked diversity in the topology. The structural and topological diversity has been analyzed from the single crystal X-ray structure. Here, in a unit, each of the two Cu(II) centres is chelated by two phenanthroline ligands and citrate (cit<sup>3-</sup>) serves the role of a bridging ligand. Furthermore, the carboxylate moiety/hydroxyl oxygen sites of citrate and the aromatic chelating ligands promote supramolecular recognition through hydrogen bonding and other non-covalent interactions (like π-π interaction) and water of crystallization, thereby resulting in a higher dimensional architecture. The oxygen atoms of the carboxylate moiety involve in both inter and intramolecular hydrogen bonding with the water molecules resulting in a hydrogen bonded helical supramolecular solid. Theoretical study is performed to analyze the structure and the role of non-covalent interactions through DFT based calculations and Hirshfeld surface analysis.

**Keywords:** Supramolecular architectures, Density functional calculations, Crystal structure, Hydrogen bonding, π-π interactions, Copper, Citrate,

Crystal engineering of coordination polymers has attracted great attention in recent years due to their potential as functional materials as well as their interesting compositions and topologies<sup>1</sup>. These hybrid inorganic/organic materials with extended frameworks are thus worth mentioning owing to their interesting structures and potential applications in sorption, gas storage, enantio-separation, catalysis, sensing and magnetism<sup>2</sup>. Detailed mechanistic study suggests that these intriguing functionalities may have originated either from the organic portion and/or from the metal centers of the coordination moiety or might be a collective contribution from both the organic and inorganic members<sup>3</sup>. Since the last decade, the synthesis of metal carboxylates has grown exponentially due to the development of a new class of hybrid inorganic-organic materials with

novel functionalities, which opened their scope of applications in the area of molecular adsorption, catalysis etc. These metal-organic frameworks (MOF) or coordination polymers have been constructed from the association of different types of metals together with different types of organic linkers<sup>4</sup>. Numerous coordination polymers have been prepared to date by the self-assembly of metal ions and multidentate ligands with various sizes and geometrical preferences. Many of these materials contain porous frameworks that mimic their inorganic counterparts, zeolites and molecular sieves, but with greater variety of sizes and shapes depending on the choice of building blocks. Although the general and precise principles for controlling the solid structures of the target products still need to be established, many rational synthetic strategies like hydrothermal,

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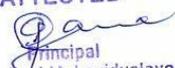
**Book Review: An(other) Quest for the Political: Ranjan Ghosh's Detechnification of Pedagogy Through Tagore**

Samrat Sengupta

While reading Ranjan Ghosh's book *Aesthetics, Politics, Pedagogy and Tagore: A Transcultural Philosophy of Education* (2017) one may follow the (in)fusion approach and the philosophy of trans introduced by Prof. Ghosh himself (Ghosh 2016). One may break the epistemic securities of ideas within their safe contours of tradition and belonging to infuse and activate other ideas – other spaces. Thus, the philosophical potentialities, the potency of philosophy or philosophical thinking as potentialities (following Agamben) would be directed towards an undecidable future – the realm of a confrontation with non-knowledge.<sup>1</sup> The future resides in the openness of possibilities of meaning that is hidden and which surfaces in the literariness of our readings. Activating ideas with other ideas would make the (in)possible meanings move from depth to the surface. Ghosh's work points towards such inadvertent hybridity of ideas. As Ghosh with his inimical style charges Tagorean ideas on pedagogy and philosophy (linked inseparably as both form together a realm of practice and also transforms the same to address the famous Marxian gap between interpretation and change in "The Thesis on Feuerbach") with his readings of thinkers across the continents (resonating with the title of his other book, co-authored with J. Hillis Miller, *Thinking Literature Across Continents*) the spectre of debates and discussions on Tagore's philosophy and its relevance in the present world surfaces, transcending the limits of his book. Ranjan Ghosh's book invites such textual and ideational transcendence and inquiry. In a recent special supplement on Tagore in *Economic and Political Weekly*, Pradip Kumar Dutta, in his introduction, comments on the "new generation of work on Tagore" after his 150<sup>th</sup> birth anniversary which focuses more on "the less familiar area of Sriniketan, the rural development wing of the global pedagogic institution that Tagore called Visva-Bharati" but which "does not leave out the more familiar world of Santiniketan, but views it from the perspective of materialist aesthetic practices" (Dutta 2017, 38) as he claims to have been done in the collection he was introducing. He also points out how in the eve of his 100<sup>th</sup> anniversary in 1961, the anniversary edition published from Sahitya Akademi "does not have a single essay on his institution-making." Ranjan Ghosh's book effectively addresses that lacuna. As he does so, writing in English for a wider global audience, his work pushes us to address a larger question of postcolonial scholarship and its politics. It becomes an addition to our postcolonial speculations on identity, marginality and thinking of the other.

This review essay would attempt to examine in the light of Ranjan Ghosh's book how far Tagore helps us to deal with the complex question of identity and marginality that disturbs and unsettles postcolonial democracies. In the traditional field of discussing the politics of Tagore he is mainly identified as a man of ideas. Those who hail him as a poet-philosopher and make him a cultural icon prefer him for his great ideas and those who are critical of him are so for his benevolent but impractical ideas. There has been a tradition of Marxist critiques in Bengal who denounced Tagore for being a bourgeois ideologue – a landlord by birth, carrying social and cultural privileges of his upper class, upper caste, and colonized bourgeois identity. While some negate him for his privileged position and the focus of his literary work being largely the middle-classes, others see his good intentions limited by his economic and ideological confines. However, Ranjan Ghosh's book ascertains Tagore's thinking as a different sort of practice – a practice that insinuates a crossing over. Prof. Ghosh does so by focusing on Tagore's prose writings and his ideas on learning, educating and pedagogy. Tagore for him is a poet philosopher as he infuses the poetic function of creation, in identity formation and knowing oneself through education. Ranjan Ghosh's book generates further possibilities of reading Tagore's philosophy as an aesthetic practice to keep open the future that is to come. Derrida's idea of *democracy to come* may become the aesthetic imaginary for self-formation in Tagore where the subject is not decidable and determinable fully by the network of power and remains open to the future while not erasing its past and present. While Derrida's work focuses on *democracy to come*, Ranjan Ghosh focuses on Tagore's ideas to show how the selves of the subjects of *democracy to come* could be created poetically. Here we may move from Derrida to Agamben to

ATTESTED 104

  
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Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

# Solvent Dependent Nanostructures Based on Active $\pi$ -Aggregation Induced Emission Enhancement of New Carbazole Derivatives of Triphenylacrylonitrile

Santu Maity,<sup>[a]</sup> Krishnendu Aich,<sup>[a]</sup> Chandraday Prodhon,<sup>[b]</sup> Keya Chaudhuri,<sup>[b]</sup> Ajoy Kumar Pramanik,<sup>[c]</sup> Siddhartha Das,<sup>[d]</sup> and Jhuma Ganguly\*<sup>[a]</sup>

**Abstract:** In the present study, the carbazole and 2,3,3-triphenylacrylonitrile (TPAN) nanostructures (2-CTPAN and 2,2'-CTPAN) have been designed and synthesized by Pd-catalyzed Sonogashira cross-coupling reaction. CTPAN exhibit aggregation induced emission enhancement (AIEE) behaviour in water with high fluorescence quantum yield. Both the compounds show tunable self-assembly in water as well as in dimethylformamide (DMF) by extended  $\pi$ - $\pi$  stacking interaction. CTPAN can be self-assembled into spherical particles in water and the structures of these self-assemblies have been investigated using X-ray diffraction. Interestingly, 2-CTPAN and 2,2'-CTPAN form organogels with a critical gelation concentration (CGC) of 11 and 15 mg/mL, respectively, in DMF and exhibit acicular and rod shaped morphology, respectively. The single crystal structure of 2-CTPAN shows that the intermolecular C-H $\cdots$  $\pi$  interactions lock the molecular conformation into a staircase-shaped supramolecular assembly. These AIEE active compounds reveal high water dispersibility, strong yellow fluorescence with high quantum yield, promising photostability and excellent biocompatibility which make them a potential bio-imaging agent.

## Introduction

The development of novel fluorescent nanoparticle based bio-imaging probes have created new avenues in interdisciplinary fields that range from biology to materials science.<sup>[1]</sup> Their remarkable optical properties make them promising for drug delivery, bioanalysis, bio-imaging and other biomedical applications.<sup>[2-4]</sup> Previously, a large number of inorganic fluorescent nanoparticles including quantum dots, silicon quantum dots, carbon dots, fluorescent metal clusters and Ln<sup>3+</sup>-ion doped nanomaterials have been extensively explored for bio/chemosensors applications.<sup>[5-11]</sup> In spite of the advantages of strong fluorescence intensity and limited dosage, fluorescent inorganic nanoparticles have many inherent disadvantages for

biomedical applications, such as relatively laborious synthesis, difficult to tune fluorescence, potential toxicity due to their accumulation in the reticuloendothelial system (RES) after intravenous injection, blinking effect, poor biodegradability and non-functionalized hydrophobic entities.<sup>[12,13]</sup> Fluorescent proteins are also a class of bioprobes which also have limited applications due to their high cost, low molar absorptivity and low photobleaching thresholds.<sup>[14]</sup> On the other hand, organic dyes and conventional fluorescent organic nanoparticles (FONs) exhibit aggregation caused quenching (ACQ) issue, poor membrane permeability and easy photo-bleaching.<sup>[15-17]</sup> Besides, the photostability is very important for protracted observation, where photobleaching rigorously affects the capability to sense the target molecules.<sup>[18,19]</sup>

Thus, novel fluorescent nanoparticles FNPs with good biocompatibility and low cytotoxicity are still in urgent pursuit.<sup>[20,21]</sup> Recent advancements on the unique aggregation induced emission (AIE) based materials open up a new opportunity for the preparation of the organic molecule based fluorescent nanoprobe.<sup>[22-26]</sup> Till date, a large number of AIE active molecules with different chemical characteristics have been discovered and utilized for fabrication of AIE-active FONs including naphthalene-diimide, tetraphenylethene (TPE), siloles, PEGylated carbazole and some metal complexes.<sup>[27-32]</sup> Such probes have been used as fluorescent tools for the detection of biomolecules and biochemical events, imaging agent in live cells, organic light-emitting devices and chemosensors.<sup>[33-35]</sup> AIE active molecules can be transformed into functionalized nanoparticles with their varied applications in biomedical field.<sup>[36]</sup> With the intention to develop AIE based nanoparticles, several approaches have been reported yet. The simplest approach is the incorporation of AIE moiety into the self-assembled/aggregated structure of the polymers or molecules and it has emerged as a fascinating aspect owing to their optimum flexibility, extensive  $\pi$ - $\pi$  interaction, and the feasibility of peripheral modification with various functional groups for enhanced intermolecular interactions.<sup>[37-39]</sup> Size of these nanoparticles have been controlled between 25 to 300 nm for successful biomedical applications.<sup>[2]</sup>

Though, there has been a significant progress in the AIE active nanoprobe, there are still several issues for their wider applications. Firstly, the presence of non-AIE molecule/polymer in the core of AIE-based nanoparticle makes its fluorescence property highly dependent on the amount of AIE molecule. Secondly, synthesis of fluorescent nanoparticle of controlled size is very difficult by these methods due to the existence of non-AIE materials. Thirdly, most of these nanoparticles have low colloidal stability and frequently lose their assembled structure. Fourthly, a very few number of functionalization has been

[a] Mr. S. Maity, Dr. K. Aich, Dr. J. Ganguly  
Department of Chemistry, Indian Institute of Engineering Science and Technology, Howrah-711103, India  
E-mail: jhumaiest@gmail.com

[b] Mr. C. Prodhon, Prof. Keya Chaudhuri  
Molecular Genetics Department, CSIR-Indian Institute of Chemical Biology, Kolkata, 700032, India

[c] Dr. A. K. Pramanik  
Department of Chemistry, New Alipore College, University of Calcutta, Kolkata, 700053, India

[d] Prof. S. Das  
Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Kharagpur, 721302, India

Supporting information for this article is given via a link at the end of the document.

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ARTICLE

## Facile detection of organophosphorus nerve agent mimic (DCP) through a new quinoline-based ratiometric switch

Saswati Gharami, Krishnendu Aich, Sangita Das, Lakshman Patra and Tapan Kumar Mondal\*

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In this paper, a quinoline-based (BIMQ) probe has been developed which displays a ratiometric detection of organophosphorus (OP) chemical vapor threat, DCP. Upon addition of the nerve agent mimic diethyl chlorophosphate (DCP), a fluorescence color change from blue to cyan was observed. The chemodosimeter (BIMQ) undergoes nucleophilic substitution reaction with DCP followed by a ring closure to yield the final product and shows a explicit fluorescence response towards DCP. The probe (BIMQ) selctively detects DCP over other toxic analytes. Now the detection limit of BIMQ for DCP was established to be in the order of  $10^{-8}$  M in solution phase which suggests that BIMQ is efficient in detecting DCP in very minute level. This ratiometric switch has a potential application as a portable kit for detecting DCP vapour with high sensitivity. TDFT calculations have been carried out in order to unveil the electronic properties theoretically.

### Introduction

Chemical warfare agents (CWAs) are comprised of nerve agents, blood agents, vesicant agents, incapacitating agents, cytotoxic proteins etc.<sup>1</sup> Among these CWAs, nerve agents are one of the most exceptional dangerous brand which has extreme harmful effects on health of every living beings if inhaled or through any kind of contamination to foods or drinks.<sup>2,3</sup> These odorless and colorless chemicals along with the advantage of their cheap and easy fabrication process possess a high risk of being used as a most dangerous tool of mass annihilation in the battle field through terrorists attacks.<sup>4,5</sup> These nerve agents are a class of chemically active and highly toxic volatile liquids or gases derived from organophosphates which are considered to be one of the most poisonous chemicals to human beings as well as to any other human beings.<sup>6</sup> Nerve agents, such as sarin (GB), soman (GD), and tabun (GA), are extremely lethal organophosphates which consists of very good leaving groups owing to which they are called essential phosphorylating and phosphonylating agents.<sup>7-11</sup> So they act as a potent inhibitors of acetylcholinesterase (AChE) in the central nervous system by irreversibly binding with the hydroxyl group of this enzyme which is mainly responsible for the hydrolysis of acetylcholine neurotransmitters.<sup>12-15</sup> The interaction of the nerve agent with AChE actually blocks the decomposition of acetylcholine. This accumulation of acetylcholine results in the neurological imbalance in the cholinergic synapse, the neuromuscular

paralysis, hindrance of muscle relaxation, organ failure, eventually leading to rapid death.<sup>16-20</sup> So due to these massive threats offered by the nerve agents in our environment, there is an utmost need of developing a reliable, facile and rapid method of detecting them distinctly. An associated compound, diethyl chlorophosphate (DCP), which has comparable reactivity and structure as compared to the real nerve agents is usually used as a nerve gas-mimic agent for scientific research purpose owing to the fact that the actual nerve agents are hard to avail and also possess too much toxic nature.<sup>21</sup>

In recent years, a variety of noteworthy methodologies for detecting the nerve agent mimics have been introduced which includes mass spectrometry,<sup>22-24</sup> electrical sensors<sup>25-27</sup>, enzyme-based biosensors,<sup>28-31</sup> use of enzymatic assays,<sup>32</sup> photoacoustics,<sup>33</sup> PET based probes,<sup>34</sup> cyclisation reactions,<sup>35</sup> ion mobility spectroscopy,<sup>36</sup> nucleophilic substitution reactions,<sup>37</sup> complex formation based probes,<sup>38</sup> lanthanide luminescence,<sup>39</sup> photonic crystals,<sup>40</sup> optical-fibre arrays,<sup>41</sup> nanomaterials (nanotubes or nanowires)<sup>42,43</sup> etc. But these methods have some disadvantages such as low specificity, inadequate selectivity, reduced sensitivity and difficulties in real-time monitoring. So the designing of small molecule based fluorescent probes is considered to be an unrivalled methods to discriminate these harmful toxic nerve agents owing to their high sensitivity and stability, low-cost, real-time monitoring, easy portability and operational simplicity.<sup>44,45</sup> The sensing mechanism of these probes mainly includes the addition of phosphoryl group of these organophosphorous nerve agents to an aromatic or aliphatic hydroxyl group,<sup>46</sup> a pyridine group,<sup>47</sup> an oxime group,<sup>48</sup> an amine group,<sup>49</sup> a spirobenzopyran group<sup>50</sup> or a carbonyl group.<sup>51</sup> Although there

Department of Chemistry, Jadavpur University, Kolkata-700 032, India.  
E-mail: tapank.mondal@jadavpuruniversity.in  
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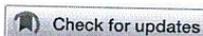
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## Simple fabrication of a carbaldehyde based fluorescent "turn-on" probe for the selective and sole detection of Pd<sup>2+</sup>: application as test strips†

Chandan Kumar Manna, Saswati Gharami, Krishnendu Aich, Lakshman Patra and Tapan K. Mondal \*

A new fluorescent "turn-on" probe (DHMC) has been designed and synthesized to selectively detect Pd<sup>2+</sup> among other cations at physiological pH. Upon incremental addition of Pd<sup>2+</sup> into the probe solution, a "turn-on" emission enhancement was noticed with a ~69 nm red shift at 562 nm in CH<sub>3</sub>CN/H<sub>2</sub>O (4/1, v/v) solution. The limit of detection and binding constant values have been determined and found to be on the order of 7.4 × 10<sup>-8</sup> M and 1.7 × 10<sup>5</sup> M<sup>-1</sup> respectively, which clearly suggests that the probe is very efficient in detecting Pd<sup>2+</sup> at very minute levels and also the DHMC-Pd<sup>2+</sup> complexation is stable enough too. A brilliant application of the probe has been explored which indicates that DHMC can detect Pd<sup>2+</sup> in the solid state too. DFT and TDDFT calculations are carried out to interpret the electronic structure and sensing mechanism.

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### Introduction

Palladium is a platinum group element and one of the most valuable transition metals. It is extensively used in a range of applications such as the jewelry business, coating materials, dental crowns and chemical catalysts.<sup>1-4</sup> Mainly, Pd-catalyzed C-C cross-coupling reactions have been renowned as competent and handy tools for the synthesis of organic compounds including pharmaceutical products.<sup>5,6</sup> However, an adverse influence of this metal on human health has created a grave concern as palladium ions can bind to thiol-containing proteins (e.g. casein and silk fibroin), DNA or other biomolecules because of their high nucleophilicity.<sup>7,8</sup> Palladium residues in pharmaceutical compounds or in the environment may cause a substantial hazard especially for environmental pollution emissions to water and soil.<sup>9</sup> Therefore, the governmental regulation on the proposed maximum nutritional intake of palladium is less than 1.5–15 µg per person per day.<sup>10</sup> Therefore, design and development of a selective and sensitive analytical method for the recognition of palladium in the environment is essential to assess possible adverse health effects caused by this particular metal residue.

The conventional techniques used for quantification of palladium species, such as atomic absorption spectroscopy

(AAS), inductively coupled plasma atomic emission spectroscopy, solid-phase micro extraction high-performance liquid chromatography *etc.*, frequently proved to be more time-consuming, and they often demand complicated sample preparation and also they are more expensive and sophisticated and thus are not so appropriate for real-time and *in situ* analysis.<sup>11</sup> So currently the fabrication of fluorescent molecular probes is among the most cultivated techniques owing to their simplicity of application in solution as well as their high sensitivity and selectivity and tunability for trace analytes.<sup>12</sup> As a result, the requirement of the development of this type of new fluorescent probes has become a vital area of research nowadays.<sup>13</sup> Although there have been some reports on Pd<sup>2+</sup> sensors recently,<sup>14</sup> our probe still shows a simple synthetic route and distinguishes Pd<sup>2+</sup> solely among other cations in acetonitrile–water medium (4/1, v/v).

So herein we have presented the design and development of a new fluorescent probe based on the carbaldehyde moiety which distinctly senses Pd<sup>2+</sup> among other metal ions, displaying a high detection limit value of 7.4 × 10<sup>-8</sup> M.

### Experimental

#### Materials and methods

2-Amino-4-methylphenol was purchased from Aldrich. All the other organic materials and solvents were purchased from commercial sources and used without further purification. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on a Bruker 300 MHz

Department of Chemistry, Jadavpur University, Kolkata - 700032, India.  
E-mail: tapank.mondal@jadavpuruniversity.in

† Electronic supplementary information (ESI) available: NMR and MS of all new compounds, limit of detection determination, quantum yield calculation. CCDC 1939357. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/c9nj04313f

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Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

## Analytical Chemistry

Two New Quinoline-Benzothiazole Blended 'Off-On' Type Fluorescent Probes Exclusively Detect  $\text{Cd}^{2+}$ Krishnendu Aich, Sangita Das, Saswati Gharami, Lakshman Patra, and Tapan Kumar Mondal<sup>\*[a]</sup>

In this paper, two new quinoline-benzothiazole based probes (QBTP1 and QBTP2) have been synthesized for the selective detection of  $\text{Cd}^{2+}$ . Both the probes showed selective 'Turn-On' emission change towards  $\text{Cd}^{2+}$ . Structure of QBTP1 was confirmed through its single crystal X-ray study. QBTP1 itself showed a weak emission band at 488 nm which upon addition of  $\text{Cd}^{2+}$  enhanced dramatically with a slight redshift to 507 nm. Consequently, weak cyan emission of QBTP1 changes to green which is easily observable through naked eyes. QBTP2 also showed almost similar fluorescence change upon addition of  $\text{Cd}^{2+}$  to that of QBTP1. The intramolecular charge transfer (ICT) and chelation enhanced fluorescence (CHEF) mechanisms may

play here the key role for this type of redshift of emission maximum and enhancement of fluorescence intensity respectively, upon addition of  $\text{Cd}^{2+}$  to the probes. Both the probes exclusively detect  $\text{Cd}^{2+}$  over any other cations tested. Most importantly, not a minute interference was observed by  $\text{Zn}^{2+}$  or  $\text{Hg}^{2+}$ . Capabilities of the probes to be used as portable kits for on-site detection of  $\text{Cd}^{2+}$  without using any expensive instrumental help was also shown here. Furthermore, the limit of detection of both the probes were found in the order of  $10^{-9}$  to  $10^{-10}$  M range which indicates the high sensitivity of the probes towards  $\text{Cd}^{2+}$ .

## Introduction

Cadmium has been recognized as a highly toxic heavy metal and is placed in the seventh position on the top twenty Hazardous Substances Priority List by the Agency for Toxic Substances and Disease Registry and the US Environmental Protection Agency (EPA).<sup>[1,2]</sup> There have been many reports on the toxicity of  $\text{Cd}^{2+}$  to the human kidney, lung, bone and nerve system, which resulted in many serious health problems such as renal dysfunction, calcium metabolism disorders and an increased incidence of certain forms of cancers.<sup>[3]</sup> The affordable level of cadmium in drinking water suggested by the WHO (World Health Organization) is 3 ppb to prevent the diseases held from cadmium toxicity.<sup>[4]</sup> In particular,  $\text{Cd}^{2+}$  can replace  $\text{Zn}^{2+}$  in many zinc enzymes, thereby impairing their catalytic activities.<sup>[5]</sup> The  $\text{Cd}^{2+}$ -uptake and carcinogenesis mechanisms are still insufficiently understood, mainly because of the lack of facile analytical methods for monitoring changes in the environmental and intracellular  $\text{Cd}^{2+}$  concentrations with high spatial and temporal reliability. Thus, the development of novel fluorescent sensors for  $\text{Cd}^{2+}$  has received considerable attention. However, it is still remaining a challenging task to design fluorescent switches for the exclusive detection of  $\text{Cd}^{2+}$ .  $\text{Zn}^{2+}$  or  $\text{Hg}^{2+}$  may interfere in the detection of  $\text{Cd}^{2+}$ .<sup>[6]</sup> So, it is being the main challenge to fabricate such type of fluorescent

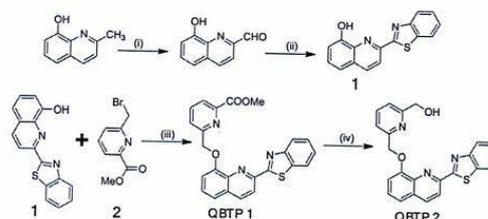
sensors which can be employed for detection of only  $\text{Cd}^{2+}$ . Therefore, tremendous efforts have been devoted for the development of fluorescence sensors which can detect  $\text{Cd}^{2+}$  without any interference from other bivalent ions.<sup>[7]</sup>

Keeping these factors in mind we have developed two new quinoline-benzothiazole blended fluorescent 'turn on' probes (QBTP1 and QBTP2), which can selectively detect  $\text{Cd}^{2+}$  in comparison to different guest analytes, especially  $\text{Zn}^{2+}$  and  $\text{Hg}^{2+}$ . The probing of  $\text{Cd}^{2+}$  was investigated by absorption, emission, <sup>1</sup>H NMR and HRMS spectroscopic techniques.

## Results and Discussion

## Synthesis of the probes (QBTP1 and QBTP2)

The synthetic scheme of the probes (QBTP1 & QBTP2) is shown in Scheme 1. Compound 1<sup>[7e]</sup> and compound 2<sup>[7d]</sup> are prepared



Scheme 1. Synthesis of the probes (QBTP1 and QBTP2). Reagents and conditions: (i)  $\text{SeO}_2$ , 1,4-dioxane, reflux, 6 h; (ii) 2-aminothiophenol, p-TSA, DMF, 60°–70° C, 12 h; (iii)  $\text{K}_2\text{CO}_3$ , DMF, TBAB, r.t., 6 h; (iv)  $\text{NaBH}_4$ ,  $\text{CH}_3\text{OH}$ , 2 h.

[a] K. Aich, S. Das, S. Gharami, L. Patra, T. K. Mondal  
Department of Chemistry, Jadavpur University, Jadavpur, Kolkata-700  
032, India

E-mail: tapanmondal@jadavpuruniversity.in

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## Anodic Oxidation of Butan-1-ol on Reduced Graphene Oxide-Supported Pd–Ag Nanoalloy for Fuel Cell Application

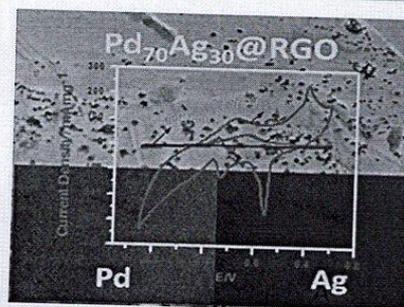
Ankita Mahajan,<sup>†</sup> Senjuti Banik,<sup>†</sup> Dipanwita Majumdar,<sup>‡</sup> and Swapan Kumar Bhattacharya<sup>\*,†</sup>

<sup>†</sup>Physical Chemistry Section, Department of Chemistry, Jadavpur University, Kolkata, 700 032 West Bengal, India

<sup>‡</sup>Department of Chemistry, Chandernagore College, Chandannagar, Hooghly, 712136 West Bengal, India

### Supporting Information

**ABSTRACT:** Reduced graphene oxide (RGO)-supported bimetallic Pd<sub>x</sub>Ag<sub>y</sub> alloy nanoparticles of various compositions were synthesized by one-pot coreduction of respective precursors with hydrazine for use in the anode catalysis of oxidation of butan-1-ol in alkali. The as-synthesized catalyst materials were characterized by microscopic, spectroscopic, and diffraction techniques. Cyclic voltammetry (CV), chronoamperometry, and polarization studies infer that a few Pd<sub>x</sub>Ag<sub>y</sub> materials exhibit an enhanced and synergistic catalytic activity in reference to Pd and Ag nanomaterials. Among the various RGO composites of Pd<sub>x</sub>Ag<sub>y</sub> alloy on graphite support, the one containing the Pd<sub>70</sub>Ag<sub>30</sub>@RGO composite is the best in catalytic activity. The cycle life of the catalyst is found to be very high, and PdO and Ag<sub>2</sub>O are found to be generated in the catalyst material with little change in the catalytic capability during the 100th cycle of CV operation. The addition of Ag upto 30 atom % in the Pd<sub>x</sub>Ag<sub>y</sub> alloy causes greater formation of butyraldehyde and butyl butanoate among the various products. Larger atom % of Pd helps to form sodium butyrate and sodium carbonate, as evident from the ex situ Fourier transform infrared and high-performance liquid chromatography study of the product mixtures and the separate CV studies of the intermediate products. A suitable mechanism is also proposed to fit the findings.



### INTRODUCTION

In the era of rapidly depleting fossil fuel and ever-rising demand for renewable and sustainable energy, the urge for environment-safe fuel source and its proper utilization has become an immediate concern for the modern society.<sup>1</sup> Direct alcohol fuel cells (DAFCs) appear as potential alternative green and renewable power devices, as these use liquid fuels, which are harmless, easy to handle, and easy to store as well as affable to the ecosystem.<sup>2,3</sup> In addition, these devices possess higher volumetric energy densities than the gaseous hydrogen counterparts, thereby becoming more popular as highly efficient, low-emissive, and soundless power sources for cars and portable electronic devices.<sup>4</sup>

Various alcohols such as methanol, ethanol, propanol-isomers, ethane-1,2-diol, and propane-1,2,3-triol have been widely investigated as potential fuels for DAFCs.<sup>5–10</sup> The reactivity of small primary alcohols on the Pt electrode surface in acid has been found to follow the order methanol > ethanol > propanol > n-butanol.<sup>5,11</sup> However, the poor alcohol cross-over across the membrane and the complex reaction mechanism lower the cell performance, and these are the major hurdles in the alcohol oxidation process in most cases.<sup>12</sup> Nonetheless, recent studies reveal that the alcohol cross-over rate is comprehensively reduced on increasing the alcohol chain length.<sup>12</sup> Moreover, a single alcohol molecule bears one oxygen atom only; thus, the full oxidation of alcohol to carbon dioxide requires additional O atom, which is provided by water

or water-adsorbed residue (OH<sub>ads</sub>) on the metal-catalyst surface. Again, the oxidation of water on the metal surface is an energy-seeking process that upraises the anodic over potential of DAFCs. Thus, the present objective lies in full oxidation of the alcohol molecule at a lower anodic potential to attain high fuel cell efficiency.<sup>5,13–15</sup>

Various other important factors such as easy availability, accessibility, price, environmentally benign, and sustainability are important criteria for selecting a suitable fuel for DAFCs.<sup>16</sup> A thorough knowledge about the kind of intermediates, the effective cell voltage, and the amount of deliverable charge per fuel molecule is necessary for the fruitful fabrication of a fuel cell.<sup>17</sup> Methanol is comparatively easier to oxidize, but toxicity, inflammability, and nonavailability of the renewable source restrict its usage in practical DAFCs.<sup>18</sup> In contrast, ethanol is nontoxic and easily processable from sugar fermentations.<sup>19–22</sup> However, the utilization of edible food-based biomass feed stock for generation of large-scale bioethanol has been a sensitive issue of significant debate in the recent days.<sup>23,24</sup> In this regard, butanol may be considered as a suitable alternative with higher energy density and better infrastructure compatibility. Currently, it is employed as a gasoline additive as well.<sup>24–26</sup> Furthermore, it is less poisonous, noncorrosive, and

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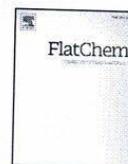
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# Temperature control synthesis of platinum nanoparticle-decorated reduced graphene oxide of different functionalities for anode-catalytic oxidation of methanol



Senjuti Banik<sup>a</sup>, Ankita Mahajan<sup>a</sup>, Apurba Ray<sup>b</sup>, Dipanwita Majumdar<sup>c</sup>, Sachindranath Das<sup>b</sup>, Swapan Kumar Bhattacharya<sup>a,\*</sup>

<sup>a</sup> Physical Chemistry Section, Department of Chemistry, Jadavpur University, Kolkata 700032, India

<sup>b</sup> Department of Instrumentation Science, Jadavpur University, Kolkata 700032, India

<sup>c</sup> Department of Chemistry, Chandernagore College, Chandannagar, Hooghly, WB-712136, India

## ARTICLE INFO

### Keywords:

Platinum (Pt) nanoparticle-decorated reduced graphene oxide  
Methanol oxidation  
Oxygen functionalities  
Defects concentration  
Temperature controlled-synthesis

## ABSTRACT

Platinum (Pt) nanoparticles of varying average diameters decorated on exfoliated reduced graphene oxide (Pt/rGO) of various functionalities have been synthesized by monitoring the temperature of co-reduction of Pt<sup>IV</sup> and GO. The as-synthesized composites are characterized by X-ray diffraction, spectroscopic, thermo gravimetric and microscopic studies. The excellent catalytic capability of the composites for methanol oxidation reaction (MOR) is found to be synergistic in reference to single components, Pt and rGO and might be used in high efficient, less emissive, cost-effective direct methanol fuel cell operated in alkali. The poison tolerance capability of the electrodes as measured by the ratio of forward and backward peak currents due to MOR is found to be relatively high in respect to similar data in the literature and increases with the increase of defect concentration as evaluated from Raman spectroscopic study, on rising the temperature of synthesis of the catalyst. The forward peak current density of the electrode made with Pt/rGO composite synthesized at 40 °C is greater by 5.6 and 287 times than these for pure Pt and rGO based electrodes. The electrode exhibits the best catalytic activity due to presence of the lowest but sufficient defect sites, especially for formation of sp<sup>2</sup>-C-OH groups on the rGO surface in the vicinity of the poisoned Pt-surface and lowest average diameter (7.41 nm) of dispersed Pt nanoparticles.

## 1. Introduction

Ever-rising demand for environmental benign sustainable energy sources has driven immense attention to direct methanol fuel cells (DMFCs), particularly for application in transportation and portable energy devices [1,2]. Methanol being a single carbon containing liquid fuel is well-studied for its simple structure, low production cost, high abundance, processability and portability [3,4]. It is inherently less prone to ignition and has high volumetric energy density (15.6 MJ/L) compared to di-hydrogen (1.91 MJL<sup>-1</sup> at 20 mPa). Moreover, it is toxic if ingested but non-hazardous in presence of reasonable safety precautions. In addition, it is stable, less volatile, and remains in liquid phase over a wide temperature range, embracing all operational criteria for fuel cells, and hence widely employed in renewable energy generation technology [5].

Platinum (Pt) is considered as one of the efficient electrocatalysts for DMFCs. However, the high fabrication prices and low stability

inhibit commercial applications of common Pt-based catalysts [6]. It is eminent that the electrocatalytic performance of a fuel cell depends highly on the composition, size, morphology and dispersion of the catalytic nano-phase [7]. The size of Pt nanoparticles is one of the most key factors influencing the performance of the catalyst [8]. Downsizing Pt nanoparticles has been identified as a profitable approach to combat the problem of low efficiency and high production cost of catalysts [9,10]. However, too small nanostructures due to large surface energy may undergo severe aggregation and adsorption [11,12] thereby inducing serious declination in their catalytic performance.

An effective strategy for solving these deactivation problems involves uniform loading of the Pt nanoparticle catalysts onto a carrier with a large surface exposure and high electrical conductivity [13,14]. Thus the support materials of catalyst play a vital role in controlling these properties. In the recent years significant research has been carried out with various carbon forms such as carbon nano tube (CNT)s, amorphous carbons, polymers as supports for the development of

\* Corresponding author.

E-mail address: [skbhata7@yahoo.co.in](mailto:skbhata7@yahoo.co.in) (S. Kumar Bhattacharya).

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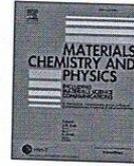
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Kolkata-700094

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## Materials Chemistry and Physics

journal homepage: [www.elsevier.com/locate/matchemphys](http://www.elsevier.com/locate/matchemphys)

## Size control synthesis of pure Ni nanoparticles and anodic-oxidation of Butan-1-ol in alkali

Senjuti Banik, Ankita Mahajan, Swapan kumar Bhattacharya\*

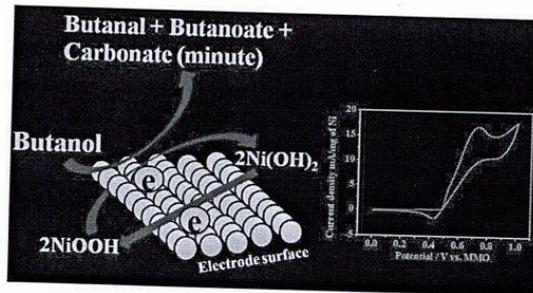
Physical Chemistry Section, Department of Chemistry, Jadavpur University, Kolkata, 700 032, India



## HIGHLIGHTS

- Ni nanoparticles of same average size are synthesized by modified polyol process.
- The maximum peak current density  $I_p$  ( $54.03 \text{ mA} \cdot \text{cm}^{-2}$ ) for BOR is obtained for Ni(4).
- $I_p$  is 14 and 2.3 times more than bulk Pt and Pd electrodes respectively.
- The best electrode can also oxidise butanal and butanoate in addition to butanol.

## GRAPHICAL ABSTRACT



## ARTICLE INFO

## Keywords:

Pure Ni nanoparticles  
Butanol oxidation  
Electrocatalysis  
Study of products

## ABSTRACT

Different sets of nickel nanoparticles with confined average diameter in the range: 9.4–13.7 nm are synthesized by varying different parameters of wet chemical method to investigate the effects of such parameters on anode catalysis in oxidation of butan-1-ol in aqueous alkali. The structure and morphology of the synthesized nanoparticles and the role of Ni and its oxides as catalyst in the oxidation of butan-1-ol have been characterized by X-ray diffractometry, scanning and transmission electron microscopy, infrared spectroscopy, cyclic voltammetry and chronoamperometry. The average particle diameter of each set is controlled by the duration of heating of precursor solution of different compositions. The required heating time and the attained maximum temperature of the reaction mixture change by changing the amount of reducing agent, solvent composition and pH of the solution. In alkali, graphite supported Ni nanoparticles form  $\text{Ni}(\text{OH})_2$  and then on application of potential  $\text{NiOOH}$  which is electro-catalytically active towards the oxidation of butan-1-ol. The catalytic activity of the as synthesized material is found to depend on the diameter of the nanoparticles, purity of the synthesized Ni nanoparticles and molecular environment around catalyst which in turn depends on the production parameters. The study reveals greater catalytic activity and increased ratio of carbonate to butanoate in the products using the pure nano-catalyst obtained by the least time of heating.

\* Corresponding author.

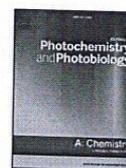
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 E.M. Bypass, Baghajatin  
 Kolkata-700094



## Synthesis of a novel pyrene derived perimidine and exploration of its aggregation induced emission, aqueous copper ion sensing, effective antioxidant and BSA interaction properties

Nilanjan Chakraborty<sup>a,b</sup>, Senjuti Banik<sup>b</sup>, Arijit Chakraborty<sup>c,\*</sup>, Swapan Kumar Bhattacharya<sup>b</sup>, Suman Das<sup>b,\*</sup>

<sup>a</sup> Department of Chemistry, Maulana Azad College 8, Rafi Ahmed Kidwai Road, Kolkata 700 013, India

<sup>b</sup> Department of Chemistry, Jadavpur University, Kolkata 700 032, India

<sup>c</sup> Department of Chemistry, Acharya B N Seal College, Cooch Behar, West Bengal 730 161, India

### ARTICLE INFO

#### Keywords:

Pyrene based perimidine  
Aggregation induced emission  
Colorimetric and turn off copper sensor  
Strong antioxidant  
Interaction with bovine serum albumin

### ABSTRACT

A new pyrene derived dihydroperimidine [2-(pyren-1-yl)-2,3-dihydro-1H-perimidine (1)] was synthesized and characterized by <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, HRMS spectroscopic techniques. The perimidine 1 was found to be a very interesting AIE luminogen with highest emission at 4:1 water-acetonitrile mixture. Compound 1 is a selective naked eye colorimetric sensor for aqueous Cu<sup>2+</sup> (colorless sensor turned brownish yellow upon contact with Cu<sup>2+</sup> ion) and gives turn off fluorescence responses in excited state spectroscopy with a limit of detection in the nanomolar range. Further it is an effective antioxidant which has been validated via 2,2-diphenyl-1-picrylhydrazyl assay and cyclic voltammetric studies in comparison to a well-known antioxidant L-ascorbic acid. To say vehemently antioxidant 1 has proven itself 5.9 times better than L-ascorbic acid. The perimidine 1 manifested interaction with protein bovine serum albumin via quenching of its own intrinsic emission intensity in Tris-HCl buffer.

### 1. Introduction

In the last few years scientists have been focusing on the development of organic luminogens exhibiting feeble emission in dilute solution whereas enhanced emission upon aggregation, i.e., aggregation induced emission (AIE) phenomenon/aggregation induced emission enhancement (AIEE) [1–10]. Fluorophores with AIE properties have found their utilities in optoelectronic and sensory systems. The AIE exhibitors are promising materials for OLEDs [11] and further fabrication of these OLEDs to electroluminescent devices [12]. They have also been accomplished as selective chemosensors, bioprobes [13–15], non-linear optical materials [16,17], logic system modulators [18] and many others.

Designing and development of chemosensors for cations and anions those are environmentally and biologically important have become an intriguing job for the present day chemist [19–26]. Cu<sup>2+</sup> demands its importance in the list amidst the biologically important metal cations being the third largest abundant transition metal ions in human body. It maintains homeostasis in human body which is exigent for the

metabolism and development [27–29]. Its pivotal role is used by many proteins in electron transport as cofactors such as superoxide dismutase, cytochrome oxidase and tyrosinase [30,31]. It catalyses redox reactions in cells, and it acts both as antioxidant, helping in reducing free radicals [32–34] as well as pro oxidant. Excessive presence of copper causes toxicity due to its catalytic activity in generation of free radicals which leads to various neurodegenerative and other diseases. Diseases like Wilson disease, Alzheimer's disease, Indian childhood cirrhosis, Menkes, and prions disease [35–38] owe their occurrence due to cellular toxicity of copper. Chronic long time exposure may result in impairment of liver and kidney. Even toxicity of Copper has its adverse effect in aquatic biota mostly in fishes and molluscs [39] among many one of which is impairment of olfactory responses in Coho salmon [40]. Due to extensive use of copper and its salts in daily lives via water pipes, utensils, wirings, medicines, fungicides, etc. contamination is very likely. Environment Protection Agency (EPA) has limited its amount to 1.3 ppm [41] which is roughly 20 μM in drinking water. Thus its detection and estimation is a high substantial matter.

The reactive oxygen species (ROS) and reactive nitrogen species

\* Corresponding author at: Department of Chemistry, Jadavpur University, Raja S. C. Mullick Road, Jadavpur, Kolkata 700 032, India.

\*\* Corresponding authors.

E-mail address: [sumandas10@yahoo.com](mailto:sumandas10@yahoo.com) (S. Das).

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Research paper

# Existence of dimeric hydroxylamine-O-sulfonic acid: Experimental observations aided by *ab initio*, DFT, Car-Parrinello and Born – Oppenheimer on the fly dynamics



Bipan Dutta<sup>a</sup>, Joydeep Chowdhury<sup>b,\*</sup>

<sup>a</sup> Department of Physics, Sammilani Mahavidyalaya, E.M. Bypass, Baghajatin Station, Kolkata 700094, India

<sup>b</sup> Department of Physics, Jadavpur University, Kolkata 700032, India

## HIGHLIGHTS

- The Raman and temperature dependent FTIR spectra of HOSA molecule have been recorded.
- Complete vibrational analyses of the molecule have been estimated from *ab initio* and DFT calculations.
- The explicit presence of D2 form of the molecule has been reveal by IR spectra recorded at high temperatures.
- The dynamics of hydrogen bonded complex formation or destruction as been estimated from the CPMD calculations.

## ARTICLE INFO

### Keywords:

Hydroxylamine-O-sulfonic acid  
FTIR  
Raman  
*Ab Initio*  
CPMD  
BOMD

## ABSTRACT

This paper reports detail study on the Raman and temperature dependent IR spectra of hydroxylamine-O-sulfonic acid molecule. Complete vibrational analyses of the molecule have been reported based on *ab initio* calculations. Raman and IR spectra captured at room temperature suggest the presence of both the dimeric D1 and D2 forms of the molecule. However, the IR spectra of the molecule recorded at elevated temperatures mark the explicit presence of the D2 form of the molecule. The theoretically simulated temperature dependent dynamic IR spectra have the capability to predict the dynamics of hydrogen bonded complex formation or destruction under external perturbation.

## 1. Introduction

While covalent bonds and electrostatic interactions are the key forces that primarily hold the atoms in molecules, non-covalent interactions especially that prevail in hydrogen (H) bonds play significant roles in various biochemical processes [1–5]. These H-bond interactions also help in promoting the necessary thermodynamic stabilities towards the formation of supramolecular and macromolecular architectures [6,7]. For example, the intermolecular hydrogen (IMH) bonds between the purine and pyrimidine bases not only embrace the DNA strands following Chargaff's rule, but also decide the orientations of the nucleotide bases amid pentose sugar and phosphate backbones. Moreover non-covalent IMH bonds also take part in the formation of molecular complexes [8,9]. The most successful and traditional ways to perceive IMH bonds in molecules have been the identification of the concerned vibrational signatures, as traced from their respective Raman and Fourier transform infrared (FTIR) spectra [10–14].

Nowadays *ab initio* molecular dynamics (AIMD) simulations play significant role to substantiate the available experimental results as obtained from Raman and FTIR spectra [15]. Born – Oppenheimer molecular dynamics (BOMD) and Car-Parrinello molecular dynamics (CPMD) are commonly applied *ab initio* molecular dynamics techniques that have been successfully used to understand the inherent dynamics involved in the H bonded molecular systems [16,17]. In BOMD calculations, the electronic energy of the molecular system is minimized and then the electronic properties of the system are estimated at each step. Within Born Oppenheimer (BO) approximation, the interaction energy in molecular dynamics calculations represents the Kohn Sham (KS) energy which in turn depends on the nuclear positions of the concerned molecular system. The potential energy hypersurface of the molecular system is thus generated from the movement of the nuclei [16].

In contrast to BOMD, the CPMD approach is based on the electronic optimization method, where a fictitious electronic mass is assigned to the propagating orbitals of the electrons. In this approach the

\* Corresponding author.

E-mail address: joydeep72\_c@rediffmail.com (J. Chowdhury).

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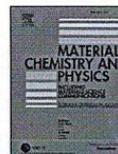
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## Selective and sensitive detection of L-Cysteine via fluorometric assay using gold nanoparticles and Rhodamine B in aqueous medium



Pradip Maiti<sup>a,b</sup>, Tanmoy Singha<sup>a</sup>, Utsav Chakraborty<sup>a</sup>, Sannak Dutta Roy<sup>a</sup>, Parimal Karmakar<sup>c</sup>, Bapi Dey<sup>d</sup>, Syed Arshad Hussain<sup>d</sup>, Sharmistha Paul<sup>b,\*\*</sup>, Pabitra Kumar Paul<sup>a,\*</sup>

<sup>a</sup> Department of Physics, Jadavpur University, Jadavpur, Kolkata, 700032, India

<sup>b</sup> West Bengal State Council of Science and Technology, Department of Higher Education, Science and Technology and Biotechnology, Vigyan Chetana Bhavan, Sector-I, Salt Lake, Kolkata, 700064, India

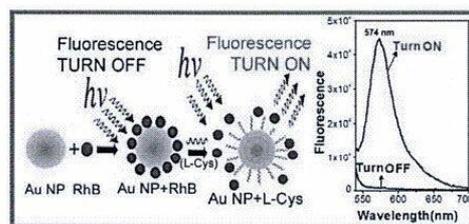
<sup>c</sup> Department of Life Science & Bio-technology, Jadavpur University, Jadavpur, Kolkata, 700032, India

<sup>d</sup> Department of Physics, Tripura University, Suryamaninagar, 799022, Tripura, India

### HIGHLIGHTS

- Gold nanoparticles can sufficiently quench the fluorescence of Rhodamine B dye.
- L-Cysteine was detected selectively from fluorescence of dye/nanoparticle mixture.
- Selective fluorescence response was accompanied with an observable color change.
- The calibration curve for the assay of L-Cysteine was almost linear.
- Selective response of L-Cysteine in real human urine sample via fluorometric assay.

### GRAPHICAL ABSTRACT



### ARTICLE INFO

**Keywords:**  
Gold nanoparticle  
Rhodamine B  
Amino acids  
Colorimetric/fluorometric  
L-cysteine  
Urine

### ABSTRACT

An assay method based on fluorometric and colorimetric change was developed for selective sensing of important thiol containing amino acid L-Cysteine (L-Cys) by using gold nanoparticles (Au NPs) and Rhodamine B (RhB) in aqueous environment. This fluorometric assay is basically relies on the competitive binding between RhB and Au NPs via electrostatic interaction as well as strong thiol(-SH)-Au NPs bonding via chemisorption. Citrate stabilized Au NPs (diameter ~27 nm) was synthesized by soft chemical method and characterized by UV-Vis absorption spectroscopy and Transmission electron microscopic (TEM) techniques. The change in non-radiative energy transfer between RhB and Au NPs are responsible for the observed drastic fluorescence quenching of RhB via FRET process. The recovery of fluorescence from the assay solution of RhB/Au NPs after addition of L-Cys was found linear over the concentration range 0.01  $\mu\text{M}$ –1000  $\mu\text{M}$  with experimental limit of detection (LOD) of 0.01  $\mu\text{M}$ . The selective interaction of L-Cys with the mixed solution of RhB/Au NPs was reflected by the color change from wine to bluish-black of the final solution. The proposed fluorometric assay method accompanied with the observed colorimetric change could successfully differentiate other interfering amino acids including thiol (-SH) containing compounds namely L-Methionine, L-Homocysteine and antioxidant glutathione with the high degree of accuracy. Also the LOD is comparable to the concentration of L-Cys present in the blood plasma.

\* Corresponding author.

\*\* Corresponding author.

E-mail addresses: [sharmistha.paul@gov.in](mailto:sharmistha.paul@gov.in) (S. Paul), [pkpaul@phys.jdvu.ac.in](mailto:pkpaul@phys.jdvu.ac.in) (P.K. Paul).

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*Pana*  
Principal  
Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
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## Study of Interaction and its Dynamics with Reference to Spotted Deer and Sambar Populations at Spatial Scales, under the Influence of Resource and Habitat Heterogeneity : A Case Study with Special Reference to Kanha and Bandhavgarh National Park

Debashis Roy, Kamonasish Mistry

Received 3 October 2018; Accepted 6 November 2018; Published on 27 November 2018

**Abstract** The Spotted deer (*Axis axis*) and the Sambar (*Rusa unicolor*) are the 2 common sympatric species that live in Kanha National Park and Bandhavgarh N. P. Central India. They are of 2 different weight categories under family Cervidae. They live in the same habitat and enjoy resources and suffer from generalist predators asymmetrically. Here we have focused on the local populations of both the S. deer and Sambar, in different location of forests, spatially apart and categorized, grouped and ranked on the basis of resource hierarchy through NDVI values. The deme structure of these 2 species show significant variation in different forest fragments. They show different degrees correlation that varies both qualitatively and quantitatively. The regression analysis with respect to the 2 populations, give a better fit model compared to when they are mixed and are not

categorically grouped and ranked accordingly. The distributions of deer and Sambar and the interaction and influence between them, show a dynamic pattern that alter with the change of forest heterogeneity and resource availability and shuffle populations and the interactions accordingly from 1 deme to the next in order to coexist. Resource partitioning, habitat niche differentiation and the predatory strategies are also additional determining factors that play parts in shaping the distribution and mutual interactions between Spotted deer and Sambar, along with habitat heterogeneity and resources.

**Keywords** Regression study, Resource hierarchy, NDVI values, Predatory strategy, Habitat heterogeneity.

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Debashis Roy\*,  
Assistant Professor in Zoology  
Department of Zoology  
Sammilani Mahavidyalaya, Baghajatin, E. M. By Pass,  
Kolkata 94, West Bengal, India

Kamonasish Mistry  
Assistant Professor in Geography  
Department of Geography  
Sammilani Mahavidyalaya, Baghajatin, E. M. By Pass,  
Kolkata 94, West Bengal, India  
e-mail : debashis675@gmail.com,  
kamonasish79@gmail.com  
\*Corresponding author

### Introduction

Kanha N. P. (longitude 80°-26'-10'' to 81°-4'-40'' E and latitude 22°-1'-5'' to 22°-27'-48'' N) and Bandhavgarh N. P. (longitude 80°-57'-30'' to 80°-06'-15'' E and latitude 23°-36'-30'' to 23°-42'-30'' N) are the 2 tiger reserve of Madhya Pradesh, Central India. Both the forest has Langur, Spotted deer, Sambar and Indian Gaur as dominant herbivore species. The popu-

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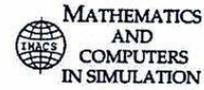
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Mathematics and Computers in Simulation 166 (2019) 432–450



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Original articles

# Pulsatile flow and heat transfer of blood in an overlapping vibrating atherosclerotic artery: A numerical study

G.C. Shit<sup>a,\*</sup>, S. Maiti<sup>a</sup>, M. Roy<sup>b</sup>, J.C. Misra<sup>c</sup>

<sup>a</sup> Department of Mathematics, Jadavpur University, Kolkata 700032, India

<sup>b</sup> Department of Mathematics, Sammilani Mahavidyalaya, Kolkata 700094, India

<sup>c</sup> Centre for Theoretical Studies, Indian Institute of Technology, Kharagpur 721302, India

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## Highlights

- Numerically studied MHD pulsatile flow of blood and heat transfer in the stenosed artery.
- Body acceleration due to vibration is considered for simulating blood flow.
- Microrotation of microparticles taken into account suspended in the porous vascular tube.
- WSS increases significantly for a rise in the permeability of the porous medium.
- Fluid acceleration enhances with an increase in amplitude of body acceleration.

## Abstract

The paper is devoted to a numerical investigation of the pulsatile flow of blood through a porous overlapping constricted artery under the influence of an externally imposed magnetic field and vibration environment that is originated from the body force. Blood is considered as micropolar fluid. The heat transfer phenomenon arising out of viscous dissipation is also studied. The problem is solved numerically by developing a Crank–Nicolson finite difference scheme after transforming the original governing equations from the physical domain to a rectangular computational domain. The computational results for the velocity and temperature distributions, fluid acceleration, skin friction and Nusselt number are presented graphically for different values of the physical parameters. The study shows that the Nusselt number increases with rise in Prandtl number and Brinkman number both and that owing to the dissipation of energy caused by blood viscoelasticity and magnetic field effect, during pulsatile flow of blood, the heat transfer rate at the wall of the artery is enhanced.

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**Keywords:** Micropolar fluid; Overlapping stenosis; Porous medium; Body acceleration

## 1. Introduction

Usually when blood flows through large arteries at a high shear rate, it can be treated as a homogeneous fluid and its flow behaviour can be described by a Newtonian model (MacDonald [20], Caro et al. [4]). Of course, Liepsch [19] carried out an experimental study to show that blood can behave like a non-Newtonian fluid, when

\* Corresponding author.

E-mail address: [gopal\\_iitkgp@yahoo.co.in](mailto:gopal_iitkgp@yahoo.co.in) (G.C. Shit).

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Kolkata-700094

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## Undecidable Spaces: Rethinking Caste and the Technologies of Abandonment in Manoranjan Byapari

Samrat Sengupta

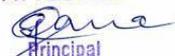
### Unfolding Space in Dalit Experience

Several attempts to understand the existence of Casteism and its manifold manifestations in Indian modernity has been made so far. Caste could be thought of as a historical as well as anthropological reality, which undergoes various transformations over time. This way of thinking can imagine the advent of modernity and its spread as a process of gradual annihilation of caste with the democratic ideals of liberty and equality slowly seeping in. It may also suggest other simultaneous factors such as the impact of colonialism or capitalism, reconfiguring and perpetuating caste hierarchies instead of their dispersion. The latter process may continue Casteism without acknowledging it in the egalitarian society that apparently believes in the democratic principles. Caste is pushed back into the unconscious of the privileged through its non-acknowledgement and unmention. The historical process of such negation could lead us towards another way of thinking caste. From diachronic analysis we may hence move towards a more structuralist analysis of caste which gets activated through a concatenation of synchronic factors working together, something that is close to what Ambedkar calls "social order".<sup>1</sup> He brings in the question of ideology in his own way, something the Marxists in the latter half of 20<sup>th</sup> century would be compelled to grapple with. Arguing the economic determinism of the Socialists of his time in 1936, he comments (much before Althusser formulated his ideas of 'overdetermination' (Althusser "Contradiction and Overdetermination" 87-127) and 'ideological state apparatuses' (Althusser "Ideology" 232-272) or the English edition of Marx's *The German Ideology* (was in circulation and discussion):

That the social order prevalent in India is a matter which a socialist must deal with; that unless he does so he cannot achieve his revolution; and that if he does achieve it as a result of good fortune, he will have to grapple with the social order if he wishes to realise his ideal—is a proposition which in my opinion is incontrovertible. (Ambedkar *Annihilation* 39)

Ambedkar defined this social order as comparable to religious discourse, which enslaves man to its propositions and injunctions, something which we may compare with the continuity of religion's false consciousness in modernity in the form of ideology, often expressed in Marx. The continuity of the religious order in modern secular India is evident as "even such things as strikes and elections, so easily takes a religious turn and can so easily be given a religious twist" (Ambedkar *Annihilation* 227). Ambedkar's assertion of the continuity of the religious within the secular could be read on one hand as the inability of Indian democracy to overcome the social order sanctioned and shaped by religious discourse. On the other hand, we can also speculate how the religious gets reabsorbed and reshaped within the structure of modernity and its own process of exploitation and alienation (Sheth 2502-2510). The apparent non-existence of caste or an erasure of the caste question could be one such appropriation by absorption of the negation, or a negation of the negation, suggesting, as if caste does not exist anymore in the modern governmental apparatus. This negation instead of being suggestive of a gradual erosion of the caste system shows its rendering unspeakable. The spaces of modernity are produced by a rarefaction of the unmodern, a pushing back and appropriation. In Indian context that

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Principal  
Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata, 700022

73 36

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## Introduction: Caste in/as Humanities: Unsettling the Politics of Suffering

Kalyan Kumar Das and Samrat Sengupta

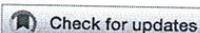
Caste, as Nicholas Dirks suggests, has become the most important and well-known register of identification of the Indian civilisation. It is often considered 'intrinsic' to the Hindu society in the scholarly investigations on India (or more generally on South Asia) emerging in the global academia (Dirks 3). From the time of early travel narratives on South Asia by western tradesmen, orientalist scholars like William Jones, Max Muller, narratives written by Christian missionaries like Charles Mead or Robert Caldwell or the denigrators of 'oriental societies' like G.W. F. Hegel and concerned critics like Karl Marx to much of our postcolonial socio-political struggles, 'caste' has been perceived as either an elusive, resilient, hydra-headed monster, or a unique feature of the Hindu society that preempts competition that western modernity brings about.

The signifier *caste*, derived from the Portuguese word *casta*, is largely a result of intercultural encounters between the 'native' social hierarchies based on endogamous units and hereditary professions on one hand, and the idea of 'purity of blood' that people of the Iberian Peninsula (Spain and Portugal) were already quite familiar with on the other (Guha 21). This complex cultural confluence that codified social hierarchies in colonial modernity, has also been portrayed as yet another 'evil colonial import' by many nationalist discourses. The traditional '*varna*' hierarchies that are found in many pre-modern so-called Hindu scriptures indeed got rigidly codified because of colonial ethnometry, ethnographic or anthropological narratives of W.W. Hunter or Herbert Risley. While the Hegelian reading of *varna* – i.e. *varna* distorted/degenerated into caste – is reiterated and popularised by many Indian nationalists, Ambedkar in his 1936 tract *Annihilation of Caste* refutes the Hegelian thesis that perceives *varna* as an experiment in social management that eventually degenerated into the present caste system (Rathore and Mohapatra 140-166).

Ambedkar debunks the *guna* theory justification of *varna* as attempted by Lord Krishna in *Bhagavat Gita* by posing a simple mathematical question i.e. if *varna* is to be deduced from the corresponding three *gunas* (*satya*, *raja* and *tamas*) originally enunciated in *Sankhyakarika*, then there has to be, mathematically speaking, three *varnas*. Moreover, in this context, Ambedkar discerns a Platonic tendency in understanding human personalities only through certain definitive and somewhat cemented characteristics. In his formulation human contingencies are neither taken into account by Plato, nor by Krishna (Ambedkar 267). Just as Ambedkar's implied critique of Plato and Hegel refutes a standardized reading of *varna*/caste, historians and anthropologists like Susan Bayly have shown that there are pre-modern/early modern or pre-colonial codifications and configurations of caste that were already getting rigidified even before colonial modernity, or its enumerative ambitions started unfolding. Therefore, this does not imply that such social features were entirely derived out of Brahminical systematization of *gunas* into caste or even determined by the colonial rule or policies. The paradigm of reading caste would, therefore, not remain confined to a simple chronological idea of history but would spread beyond the ontopological (Derrida 102-103) determinations.

Caste has undergone various forms of enframing (Heidegger 311-340) in various historical moments in the sub-continental culture which appropriates and restructures the past, instead of either abandoning or simply replicating its earlier forms. Therefore, caste could be read both diachronically as well as synchronically, as a historical formation as well

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*[Signature]*  
Principal  
Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

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## A fluorescent "ON–OFF–ON" switch for the selective and sequential detection of Hg<sup>2+</sup> and I<sup>−</sup> with applications in imaging using human AGS gastric cancer cells†

Saswati Gharami,<sup>a</sup> Krishnendu Aich,<sup>b</sup> Paramita Ghosh,<sup>b</sup> Lakshman Patra,<sup>a</sup> Nabendu Murmu<sup>\*b</sup> and Tapan K. Mondal<sup>†a</sup>

A new fluorescent "on-off-on" probe (BIPQ) is designed and developed which selectively binds with Hg<sup>2+</sup>; its emission intensity is quenched almost 40-fold at 455 nm without interference from other metal cations. On gradual addition of I<sup>−</sup> to the solution of BIPQ–Hg<sup>2+</sup>, the emission reverts to its original intensity. The limits of detection of BIPQ for Hg<sup>2+</sup> and I<sup>−</sup> are found to be on the order of 3.12 × 10<sup>−9</sup> and 5.48 × 10<sup>−8</sup> M, respectively, which shows clearly that BIPQ can sense Hg<sup>2+</sup> at a very minute level. DFT and TDDFT studies are conducted with the probe to establish similarity between theoretical and experimental outcomes. Finally, to demonstrate its practical benefit in biological fields, live cell imaging experiments with BIPQ are carried out to detect Hg<sup>2+</sup> in human AGS gastric cancer cell lines.

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### Introduction

In current research, the design, development and implementation of fluorescent chemosensors has recently gained massive interest due to their specific and nondestructive responses as well as their facile monitoring of bioactive cations and anions in different biological, environmental, toxicological and industrial samples. They are also useful in molecular devices, nerve gas sensors, *etc.*<sup>1,2</sup> The precise fluorescence responses of these chemosensors have received a great deal of attention due to their easy-to-handle characteristics, low cost and rapid discovery of target analytes.<sup>3</sup> The developed chemosensors show specific sensing towards their target molecules *via* quenching, enhancing or ratiometric shifting of their emission maxima, which facilitates rapid detection. The detection of toxic heavy metal ions has recently become very important due to their high accumulation in water and food, which frequently leads to various dangerous diseases in living beings.<sup>4</sup> Among all cations and anions, Hg<sup>2+</sup>

is one of the most detrimental and widespread heavy metal ions found in our flora and fauna.<sup>5</sup> Mercury, which is known to be a 'liquid metal' in its native form, can cause permanent damage to DNA and the nervous system if exposed or inhaled in high quantity.<sup>6</sup> The Environmental Protection Agency (EPA) has set a maximum allowable level of 2 ppb (10 nM) for mercury contamination in food and drinking water.<sup>7</sup> Inorganic mercury can be converted to methyl mercury by bacteria; this substance can bioaccumulate in the food chain<sup>8</sup> as well as in the human body, leading to various cognitive and motor disorders along with pulmonary edema, cyanosis, nephritic syndrome and Minamata disease.<sup>9</sup> Thus, there is still high demand for mercury detection methodologies for sensitive and appropriate recognition as well as hazardous assessment. Therefore, it is highly desirable to develop a powerful and sensitive analytical tool for the detection of Hg<sup>2+</sup> in environmental samples. There are few reports of fluorescent probe–Hg<sup>2+</sup> ensembles that sense iodide.<sup>10–27</sup> Among biologically significant anions, iodide is one of the most important because it is a vital micronutrient that plays essential physiological roles in human development.<sup>28</sup> Specifically, excessive iodine intake as well as deficiency can lead to thyroid disease because iodine plays an essential role in thyroid gland function.<sup>29</sup> Low iodine intake generally results in hypothyroidism, endemic goiter cretinism, congenital anomalies, neurological disorders and intellectual disability.<sup>30–35</sup> Iodine also exhibits anti-inflammatory and anti-oxidative activities.<sup>36</sup> Moreover, elemental iodine has often been used in numerous areas of chemistry for synthesizing drugs, dyes, *etc.* Generally, reported chemosensors are

<sup>a</sup>Department of Chemistry, Jadavpur University, Kolkata-700032, India.  
E-mail: tapank.mondal@jadavpuruniversity.in

<sup>b</sup>Department of Signal Transduction and Biogenesis Amines (STBA),  
Chittaranjan National Cancer Institute, Kolkata-700026, India.  
E-mail: nabendu.murmu@cnci.org.in

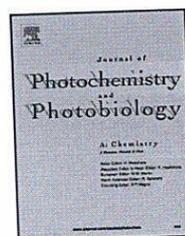
†Electronic supplementary information (ESI) available: NMR and MS of all new compounds, limit of detection determination, quantum yield calculation *etc.* CCDC 1914359. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/c9dt04245h

17 39

## Journal Pre-proof

A simple coumarin based "fluorescent On" probe for the selective detection of  $Al^{3+}$  along with its application in live cell imaging via AGS cell line

Saswati Gharami, Krishnendu Aich, Paramita Ghosh, Lakshman Patra, Nabendu Murmu, Tapan Kumar Mondal



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A simple coumarin based “fluorescent On” probe for the selective detection of  $Al^{3+}$  along with its application in live cell imaging via AGS cell line

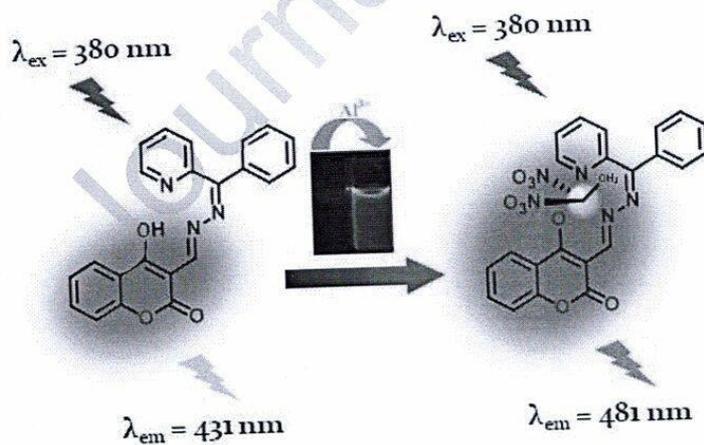
Saswati Gharami <sup>a</sup>, Krishnendu Aich <sup>a</sup>, Paramita Ghosh <sup>b</sup>, Lakshman Patra <sup>a</sup>, Nabendu Murmu<sup>b,\*</sup> [nabendu.murmu@cnci.org.in](mailto:nabendu.murmu@cnci.org.in) and Tapan Kumar Mondal<sup>a,\*</sup> [tkmondal@chemistry.jdvu.ac.in](mailto:tkmondal@chemistry.jdvu.ac.in)

<sup>a</sup>Department of Chemistry, Jadavpur University, Kolkata-700032, India.

<sup>b</sup>Department of Signal Transduction and Biogenesis Amines (STBA), Chittaranjan National Cancer Institute, Kolkata- 700026, India.

\*Corresponding author: Ph: 91-033-24572970; (TKM): (NM)

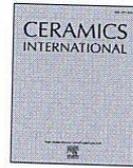
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38



# Synthesis of $\alpha$ - $\beta$ $\text{Bi}_2\text{O}_3$ heterojunction photocatalyst and evaluation of reaction mechanism for degradation of RhB dye under natural sunlight



Kamal Kanti Bera, Malay Chakraborty, Mousumi Mondal, Senjuti Banik, Swapan Kumar Bhattacharya\*

Physical Chemistry Section, Department of Chemistry, Jadavpur University, Kolkata, 700032, India

## ARTICLE INFO

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Reaction mechanism

## ABSTRACT

A few biphasic nano composites containing  $\alpha$  and  $\beta$   $\text{Bi}_2\text{O}_3$  of varying composition were synthesized by facile solvothermal method without using any capping agent and further calcination. X-ray diffraction, microscopic and spectroscopic techniques were employed for characterization of the as synthesized catalysts which are used as photocatalysts in degradation of pollutant, Rhodamine B (RhB) dye. The band gap of the nanocatalysts as calculated from tauc plot varies within 2.35–2.58 eV for  $\beta$ -form and 2.85–3.19 eV for  $\alpha$ -form in the  $\alpha$ - $\beta$   $\text{Bi}_2\text{O}_3$  heterojunctions. The operational parameters that influence the degradation process were optimized. The best catalyst dosage and pH are 0.5  $\text{g L}^{-1}$  and 4 respectively and the best concentration of  $\text{H}_2\text{O}_2$  when added is 2 mM for 10 ppm aqueous solution of dye. Among different heterojunctions, the best catalyst which is produced from bismuth nitrate concentration of 0.05 M, degrades RhB up to 99.6% at pH 4 under 120 min sunlight irradiation. The effects of addition inorganic salts in RhB dye solution were also examined. The radical trapping experiments have been applied to explore the involved and main species responsible for degradation. The identification of degradation products of RhB was analyzed and the plausible mechanistic pathway is drawn from HPLC and HRMS. It shows that the degradation of RhB proceeds via initial generation of N-deethylated products followed by ring opening ones, which indicates the photosensitization induced photocatalytic mechanism of the reaction.

## 1. Introduction

In heterogeneous photocatalysis, advanced oxidation process (AOP) has been extensively used as an eco-friendly, cost-effective and green process for productive degradation of various harmful organic pollutants [1,2] and provides solution to water quality problems. Among the various AOP, coupling of two semiconductors with different band gaps is a well-advocated strategy which increases the absorption and decreases the electron-hole recombination process. Semi-conductors like  $\text{TiO}_2$ ,  $\text{ZnO}$ ,  $\text{Bi}_2\text{O}_3$ ,  $\text{NiO}$  [3–6] etc are usually used in AOPs. Extensive research was done on  $\text{TiO}_2$  due to its high abundance, low cost and good stability. However high band gap ( $E_g$  3.2 eV) and poor absorption of sunlight (4–5%) [7] limit its performance. Therefore visible light active photocatalyst,  $\text{Bi}_2\text{O}_3$  having lower band gap (2.4–2.9 eV) is chosen [8] as an alternative. Among six main crystallographic polymorphs,  $\alpha$  (monoclinic),  $\beta$  (tetragonal),  $\gamma$  (cubic bcc),  $\delta$  (cubic face centered),  $\epsilon$  (orthorhombic),  $\omega$  (triclinic), the first one is stable at low temperature, the last one at high temperature and others are metastable state [9]. A few researches on photocatalytic activity of  $\alpha$ - $\beta$   $\text{Bi}_2\text{O}_3$

heterojunctions are summarized in Table 1 [10–17] and illustrate their importance. The table shows that the degradation efficiency of the toxic and carcinogenic dye, Rhodamin B (RhB) in natural sunlight was presented by only two previous works [12,15]. In our previous work [12], the dependence of synthesis temperature on the composition  $\alpha$ - $\beta$   $\text{Bi}_2\text{O}_3$  nano heterojunction and synergistic effect on degradation of RhB over  $\alpha$  or  $\beta$   $\text{Bi}_2\text{O}_3$  in sunlight were studied and the maximum efficiency was found to be 99.7%. In the present paper, we synthesize different  $\alpha$ - $\beta$   $\text{Bi}_2\text{O}_3$  heterojunctions by varying molar concentration of the precursor bismuth nitrate, studied their photocatalytic activity, optimize some degradation parameters like pH, effective catalyst dosage in details and the effect of addition of  $\text{H}_2\text{O}_2$  and inorganic salt like  $\text{Cl}^-$ ,  $\text{NO}_3^-$ ,  $\text{SO}_4^-$ ,  $\text{CH}_3\text{COO}^-$  in sunlight. The degradation intermediates of RhB by  $\alpha$ - $\beta$   $\text{Bi}_2\text{O}_3$  photocatalyst in natural sunlight were also identified with assistance of high resolution mass spectroscopy (HR-MS) and high performance liquid chromatography (HPLC) study.

\* Corresponding author.

E-mail address: [skbhatt7@yahoo.co.in](mailto:skbhatt7@yahoo.co.in) (S.K. Bhattacharya).

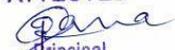
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E.M. Bypass, Baghajatin  
Kolkata-700094

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67

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## Species Habitat relationships of spotted deer through Geo-Spatial analysis at Kanha National park: A cluster oriented study

Kamonasish Mistry and Debashis Roy\*

*Assistant Professor in Geography, Assistant Professor in Zoology,  
Department of Geography Department of Zoology,  
Sammilani Mahavidyalaya, Baghajatin, E.M. By Pass, Kolkata- 94, West Bengal, India.*

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### ABSTRACT

The SAD (Species Abundance Distribution) and SDMs (Species Distribution Models) of species are important to understand the species habitat relationships. The major herbivores which are the primary prey of tigers and leopards in the tiger reserves are of special interest. In the present study we have focused on spotted deer (*Axis axis*) clusters of different size to understand the species habitat relationship in Kanha N.P. Distribution of Spotted deer were tracked by analyzing satellite images of forest patches and GPS enabled photographs of spotted deer clusters. The habitat heterogeneity of the forest and its roles in the distribution of the spotted deer clusters were determined. Major determining factors like elevational variations, stream drainage system, types of forests covers and land use; those contribute towards spotted deer distribution were also considered. Forest types of different NDVI values were found to have dynamic impact on the spotted deer population & distribution. It was also found that the spotted deer clusters of different sizes have reasonable impact on the habitat herbivores relationships. Therefore it is suggested that conservation of forest types with respect to the spotted deers are to be done considering different cluster sizes of spotted deer populations. Special attentions are to be given on the cluster specific analysis while framing the species habitat relationships, SDMs and SAD for a comprehensive and realistic outcome. In tiger reserves like Kanha national park, such practices are highly recommended for the conservation of habitats, spotted deers and the major generalist predators like tigers and leopards.

*Key words: Conservation, Resource, NDVI values, Foraging behavior, Habitat heterogeneity, Cluster analysis*

### Introduction

Spotted deer (*Axis axis*) is one of the most abundant members of the family Cervidae that shows a wide distribution range from America (South and north), Europe and Asia. It is absent in Australia, Antarctica and most of the Africa (Nayak and Sukla, 2011). The spotted deer is distributed throughout India (Nayak and Sukla, 2011) and found to be the most preferred prey species for the tiger and leopards (Sunquist,

1995). It is best seen at some of the National parks in India of which the Kanha N.P is our prime target forest.

Kanha national park is located in Madhya Pradesh, central India. It extends from 80°-26'-10" to 81°-4'-40" in longitude and 22°-1'-5" to 22°-27'-48" in latitude (Nayak and Sukla, 2011). It is surrounded by Maikal Hills and composed of grasslands and plenty of water bodies and dense forest vegetation. Rugged land scape, flat- top hills, and

Corresponding author email: debashis675@gmail.com

ATTESTED  
*Dana*  
Principal  
Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

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## **GEOSS: an intelligent methodology for identifying site suitability of air sample collection**

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### **Kamonasish Mistry**

Department of Geography,  
Sammilani Mahavidyalaya,  
Baghajatin, Kolkata, India  
Email: kamonasish79@gmail.com

### **Biplab Biswas**

Department of Geography,  
The University of Burdwan,  
Burdwan, India  
Email: biswas.biplab@gmail.com

### **Siwen Zhang**

School of Economics & Management,  
Tong Ji University,  
Shanghai, China  
Email: zsw5042@126.com

### **Tao Wu\* and Liang Zhou**

Shanghai Jiao Tong University School of Medicine,  
Shanghai, China  
Email: ijista@aliyun.com  
Email: wenzhou6@sjtu.edu.cn  
\*Corresponding authors

### **Abdelfettah Benchrif**

National Centre for Nuclear Energy, Sciences and Technology  
(CNESTEN), Morocco  
Email: abenchrif@gmail.com

### **Srimanta Gupta**

Department of Environmental Science,  
The University of Burdwan,  
Burdwan, India  
Email: srimantagupta@yahoo.co.in

**ATTESTED**  
*Pana*  
Principal  
Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

**Abstract:** Air pollution (AP) types and levels change with changes in land use land cover (LULC) types. However, there is no such attempt to develop any common methodology or model for optimum sampling which can be correlated between LULC types and changes with the AP level types and changes. A pre-planned, well-calculated geospatial method is needed to evaluate the ambient AP level, type and its variation over different LULC types. 'GEOSS' (*geospatial estimation of optimum sample site*) has been innovated to identify the optimum AP sampling sites so that it can represent the wide spatial coverage over varied LULC types. Classified satellite images and statistical tools are used to optimize sampling locations. Validation approach based on nearest neighbour analysis (NNA) has justified that GEOSS employed sampling points are systematically distributed and fulfilled all the basic assumptions of the present sampling procedure.

**Keywords:** geospatial estimation of optimum sample site; GEOSS; geospatial modelling; optimum location; land use land cover; LULC; Kolkata Metropolitan Area; KMA; air pollution level and change; sampling techniques.

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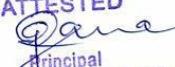
**Biographical notes:** Kamonashish Mistry is currently working as an Assistant Professor of Geography in Sammilani Mahavidyalaya under University of Calcutta, West Bengal, India. His current areas of research include air pollution, land use land cover changes and public health using remote sensing and GIS. Other areas of interest are drainage mapping and soil mapping of Rarh Bengal, India.

Biplab Biswas is a 'Raman Fellow' (USA) and Professor in the Department of Geography, The University of Burdwan, Burdwan, India. He received his PhD from the University of Burdwan in 2008. He is interested to study the environment and public health with particular emphasis on air and water quality. He uses GIS intensively in his teaching and research. He has successfully guided five PhD candidates and two MPhil candidates.

Siwen Zhang received her Masters degree in 2011 from Donghua University, and currently a PhD candidate in School of Economics and Management, Tong Ji University. Her research interest includes machine learning, artificial intelligence and their applications.

Tao Wu currently serving as a Professor in Shanghai Jiaotong University, School of Medicine. His research interests include artificial intelligence and its applications. In recent years, he has published more than 50 research papers and presided more than 20 scientific research projects at provincial level or above.

Liang Zhou received his PhD in Management Science in 2012 from Donghua University, Shanghai, China. Currently, he is serving as an Assistant Professor in Shanghai Jiaotong University, School of Medicine. His research interests include optimisation computing, simulation, modelling, and artificial intelligence.

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 Principal  
 Sammilani Mahavidyalaya  
 E.M. Bypass, Baghajatin  
 Kolkata-700094

74

46

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## Technification of Knowledge and Knowledge as Technology: the University as the Verse to Come

Samrat Sengupta

Assistant Professor and Head, Department of English, Sammilani Mahavidyalaya.

Email: [samrat19802003@yahoo.co.in](mailto:samrat19802003@yahoo.co.in)

### Abstract:

In the very act of pronouncing the word Uni-Versity the uni- in university motivates the versity – the becoming of the verse as memory – as the act of foregrounding knowledge and its continuity in time – the ontology as well as epistemology of culture and society. But at the same time the uni- is in conflict with the verse making – the versity. This double gesture produces the space of the university as an impossible, contingent and precarious space of learning. So the outside of the university is connected – hyperlinked to its inside space. If the university is made into a decided space of providing information and skill then it ceases to be a university. The erosion of liberal humanist university gradually being overcome by technological skill based universities announces the end of university. This paper shall talk about the transformative potentialities of the verse – the possibilities of unexpected turn that cannot be overcome by any technification and enframing. I would discuss university as a dialectics of desire for unification on one hand and the dynamic creative potentiality on the other that ceaselessly challenges and overcomes that unitary impulse. The idea of the University here has been discussed through the critical theoretical interventions in Jacques Derrida and Bernard Stiegler.

**Keywords:** Artifactuality, Stupidity, University, Information-Power, Enframing

The word University has close and cognate relationship with allied words such as universe and universal. Universe becomes a noun meaning “the whole world, the cosmos, the totality of things” derived from Latin *universum* in around 1580s as the noun form of the adjective *universus*. *Universus* means “relating to one”, or more literally “turned into one”. It came from *unus* (from pie root *oi-no* meaning “one” or “unique”) and *versus*, the past participle of *vertere* meaning “to turn, turn back, be turned; convert, transform, translate; be changed” (from pie root *wer* meaning “to turn, bend”). While pronouncing the word university and its deep inalienable relationship with the idea of the “universal” we often ignore the possibility of the paleonymic recurrence of its earlier traces. In the process of ascribing oneness to the hyphenated difference between the *uni* and the *versus*, the undecidable fuzzy horizon of the ‘turn’ – the precarious movement from ignorance to understanding and the versification of the world into meaning is often forgotten.

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# Fabrication of a new fluorogenic probe for detection of phosgene in solution and vapor phase

Lakshman Patra, Krishnendu Aich, Saswati Gharami, Tapan Kumar Mondal \*

Department: Chemistry, Jadavpur University, Kolkata 700032, India

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Fluorogenic chemosensor  
Detection of phosgene  
PET  
Vapor phase detection  
DFT

## ABSTRACT

A new fluorogenic probe, COUBM (where, COUBM = 3-(1H-benzoimidazol-2-yl)-8-benzothiazol-2-yl-chromen-2-ylideneamine) is designed and synthesized for selective and rapid detection of phosgene both in solution and gas phase. COUBM reacts with phosgene to form a cyclic carbamylated product (COUBM-PHOS) and consequently a sharp increase in fluorescence intensity is observed. The probe is efficiently used to detect phosgene in vapor phase using the COUBM loaded filter paper kit. Theoretical calculation by DFT/B3LYP/6-31+G(d) method is performed to interpret the electronic structure and the probable sensing mechanism of the probe for the detection of phosgene.

## 1. Introduction

Phosgene is one of the worst fatal chemical warfare gas (CWA) used in World War I [1–4]. CWAs are classified in various types such as nerve agent, pulmonary agent, asphyxiant and blister agents [5]. Phosgene is a toxic pulmonary agent. Initially, it causes eye, nose, throat and respiratory irritation. Exposure of 90 ppm of phosgene for 30 min is lethal, can cause noncardiogenic pulmonary edema, pulmonary emphysema and finally leads to death [6–12]. All the CWAs like Sarin, Soman, Tabun are strictly prohibited, unlike phosgene, due to its versatile use in industrial purposes. It is an important precursor for the production of pesticides, insecticides, pharmaceuticals, isocyanate based polymer, and aniline dyes, etc [13,14]. Due to its ready availability, it is a potential threat of terrorist attack to all mankind. Devastating annihilation can also occur from industrial leakage of phosgene. Therefore, it is very important to develop a kit for urgent alert of this threat.

Gas chromatography can be used for accurate detection of phosgene, but due to its very bad portability, a low cost, portable, highly selective and highly sensitive detection engine must be needed. There are very few publications worked on the detection of phosgene till now. Usually, these are based on nucleophilic substitution of phosgene by an amine and hydroxyl group-containing molecular probe [15–20]. Reacting with phosgene, generally, they form a cyclic compound inhibiting the photoinduced electron transfer of fluorescence quenching, to induce the emission property. Some of the groups also reported their chemosensors based on fluorescence resonance transfer [21], opening of the

amino-containing spiro (deoxy) lactum [22], conversion of cinnamic acid to coumarins [23] processes.

In the present work, we have designed and synthesized a highly selective, sensitive fluorogenic chemosensor, based on nucleophilic substitution of the probe to the electrophilic phosgene to form a carbamide molecule. The probe is named as COUBM after its precursor coumarin and benzimidazole derivative. It is very selective for phosgene over various acyl chlorides and nerve agent mimics. Vapor phase detection of phosgene is also tested by test kit made of filter paper immersed with COUBM solution. All of these tests permit the probe for onsite detection of phosgene.

## 2. Experimental

### 2.1. Material and methods

All the essential chemicals are bought from Sigma Aldrich and utilized for synthesis of the probe without purifications. Elemental analysis of the probe was carried out by a 2400 Series-II CHN analyzer, Perkin Elmer, USA. Waters (Xevo G2 Q-TOF) mass spectrometer was used for the spectrometric studies of the probe and its adduct. An infrared spectrum of the probe was recorded from RX-1 Perkin Elmer spectrophotometer by preparing KBr pellet of the sample. UV-vis absorption studies were carried out on a PerkinElmer Lambda 750 spectrophotometer. Luminescence properties were observed by Shimadzu RF-6000 fluorescence spectrophotometer at room temperature (298 K). <sup>1</sup>H and

\* Corresponding author.

E-mail address: tapank.mondal@jadavpuruniversity.in (T.K. Mondal).

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Kolkata-700094



## A GLIMPSE INTO SWAMI VIVEKANANDA'S PHILOSOPHY OF RELIGION

□ Bibek Manna\*

### ABSTRACT

Swami Vivekananda's universal religion is based on the *Advaita Vedānta*. It is known as practical Vedanta in the sense that it is grounded on the application of this universal unity of all creatures in practice. This is also the logical ground for inter-religious and intra-religious dialogue for socio-religious harmony. It is based on the Self as universal and religious way of life based on this. This attitude permits any person to have a choice of adhering to any religious faith. It does not preach uniformity. On the contrary, it appeals to universality. No religion obviously can have 'the monopoly to holiness, purity and truth.' Harmony among religions is a necessary condition for peace in society. In the absence of religious harmony and peace in a multi-religious society, there cannot be any sustainable development and in the absence of sustainable development, there cannot be prosperity.

**Keywords :** Advaita Vedānta, Phenomena, Universal Brotherhood, multiculturalism, Existence (*sat*), Consciousness (*cit*), Bliss (*ānanda*), Universal Religion.

#### Introduction :

Swami Vivekananda, the great religious teacher of modern India, introduces contemporary features to the age-old notion of religion. The present paper is a cursory discussion of his philosophy of religion. The discussion is divided in three parts. The first section devoted to his idea of religion in general. The second section consists of a brief exposition of his concept of a universal religion. The third section is devoted to the new orientation, he has suggested, to the rich philosophy of *Advaita Vedānta* to guide and control the life-pattern of modern man.

#### I

#### Vivekananda's Idea of Religion

Religion, according to Swami Vivekananda, is a basic necessity of life. Man, the strongest being in the animal kingdom, has an aspect higher than his animal self. His rationality discovers the limitations of his reason and senses. Vivekananda envisages that religious consciousness originates in mortal man's endeavor to transcend these limitations. This urge is a growth from

within and, being inherent in the very nature of man, it is universal. It is present even in an atheist, for the tendency to avoid religious ideas may also be considered as a form of religion.

Swami Vivekananda analyses religious consciousness to unravel the true nature of religion. Like all mental phenomena, religious consciousness contains three basic elements of cognition, conation and volition. Different religious sects have emphasized on one or the other of these elements. In an ideal religion these elements are to be harmonized and organized in the form of a unity.

Another unique feature of religion, according to Swami Vivekananda, is the fact that religious consciousness has a supernatural reference- be it a personal God, an impersonal absolute, a moral law or the ideal of humanity. The religious facts, unlike the scientific facts, are abstract; in every religion 'there is an ideal unit abstraction, which is put before us...'

The history of mankind has records of many

\*Research Scholar - Department of Philosophy, Calcutta University

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28 59

**THE UNION OF THE FINITE AND THE INFINITE-  
IN THE PHILOSOPHY OF RABINDRANATH**

□ Bibek Manna\*

**ABSTRACT**

As a poet and artist, Rabindranāth Tagore always aspired towards the realization of the transcendental personality of man, which he believed is immanent in the finite self only. In his writings, he laid stress on the realization of unity between the individual and the Universal Being through a perfect relationship. With Tagore, “religion” is the ultimate awakening of man's ego-consciousness in the Universal Consciousness. It is a process of realizing the Infinite 'I' in the finite 'I', by the freedom of mind and creative activities, for the goodness of humanity at large. The aim of this paper is to bring out Tagore's bifocal idea of the Self – the finite and the Infinite, his idea of humanism, Universal Man and his very own way of discovering the “religion of man”.

**Keywords :** Self; Religion of man; Tagore; Universal Man; finite; infinite; humanism.

**Introduction :**

Rabindranath Tagore (1861–1941), a revered Bengali poet, lived during a pivotal moment in history when the flow of ideas, people, and people of different faiths and civilizations grew even more linked. The decreased space between people as the world moved faster made people more prone to explosive and violent outbursts. When nations asserted their exclusive dominance and sovereignty over land, people, and the planet, however, some nations created walls while others built bridges. At that time, a voice from Bengal shouted of yoga, union, and the global religion of man.

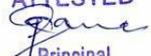
In essence, an interconnected world is captured in Tagore's works. Both external inquiry and personal discoveries are combined in his poems. The enchanting dance between the unfathomable infinite and the completeness of the finite is celebrated in his songs. His books, plays, and other writings provide insight into a life that was always in flux, one that accepted change while relentlessly pursuing the perfection of truth. For Tagore, in a world on the verge of division, unity had to be accomplished by a process of creative meditation on the

sublime—of coming to one's spontaneous self-realization—rather than by identification with that which is fleeting, such as the nation or state.

Gitanjali is by far Tagore's most well-known work in the West. He was the first non-European to win the Nobel Prize for Literature in 1913 with this collection of 103 poetry. In the foreword to the book, W.B. Yeats makes the observation that Gitanjali seems to have taken up into this imagination a whole people, a whole civilization, immeasurably strange to us; and yet we are not moved because of its strangeness, but because we have met our own image. In fact, a sense of universal searching seems to emanate from the words heard in his “song offerings. These phrases are meant to capture and preserve the divine self-awareness of the all-pervading deity alone. Three outstanding poems that were chosen from Gitanjali's beginning, middle, and end can be used to evaluate this trajectory.

For the straightforward, antagonistic reason that my interpretation of Tagore's ideas differs significantly from his, I have taken the title from the most well-known contemporary Indian philosopher. It would be impossible

\*Research Scholar - Department of Philosophy, Calcutta University

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## Effect of montmorillonite clay on the fluorescence resonance energy transfer between two cationic dyes Acridine Orange and Rhodamine B in solution

Utsav Chakraborty, Pradip Maiti, Tanmoy Singha, Ujjal Saren, Alapan Pal, Pabitra Kumar Paul\*

Department of Physics, Jadavpur University, Jadavpur, Kolkata 700032, West Bengal, India

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### ABSTRACT

In this article the Fluorescence resonance energy transfer (FRET) between two important cationic dyes namely Acridine Orange (AO) and Rhodamine B (RhB) in aqueous solution in presence and absence of montmorillonite (MMT) is demonstrated. The energy transfer is also studied in ethanolic solution. Excited state energy migration is occurred from AO to RhB molecules and the extent of energy transfer efficiency linearly increases with increase in RhB concentration in the solution. Interestingly the incorporation of MMT clay significantly increases the energy transfer efficiencies between the dye pair in the solution but the nature of interaction depends on the clay concentrations studied in the present work. The nature of quenching of steady state fluorescence emission of AO in presence of RhB as well as MMT clay in the mixed ensemble is systematically investigated and further confirmed by Time-resolved fluorescence and temperature-dependent steady state fluorescence emission experiments. AO and RhB dye molecules formed ground state complex with MMT clay followed by static quenching. As the clay platelets successfully control the FRET efficiency and it is also well known that MMT clay can host wide diversity of molecular species therefore, the present studies may provide a new insight for the design and the development of FRET-based molecular sensors.

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### 1. Introduction

Fluorescence or Förster resonance energy transfer abbreviated as FRET is an excited state photophysical process which has widespread interest to explore many biological system as well as various molecular recognition processes [1]. It was first described in 50 years ago [1] and recently has drawn great attention among the researchers in various fields of research [2–4]. FRET is a distance-dependent phenomenon by which energy is transferred non-radiatively from an electronically excited molecular fluorophore (donor) to another neighbouring fluorophore (acceptor) by means of intermolecular long range dipole–dipole coupling [5]. That is an oscillating molecular dipole can interact and exchange energy with another dipole having similar resonance frequency. The FRET can be an accurate measurement of molecular proximity at angstrom order distance i.e. 10–100 Å [6]. The extent

of this energy migration between the molecular fluorophores also depends on various parameters namely nature of solvent, microenvironment such as pH, ionic concentration, temperature etc. [7–9]. However, the main pre-requisite for FRET to occur is the sufficient spectral overlap of absorption spectrum of the acceptor and emission spectrum of the donor molecules.

Various interesting nanomaterials play significant role for the control of FRET efficiency between organic materials such as dye molecules [10]. Among those, clay nanoplatelets are already attracted great interest in this direction [7]. These are the inorganic nanolaminates which belong to the smectite group of materials and are most abundant in nature. Clays possess high surface to volume ratio, high cation exchange capacity (CEC) and can support a wide variety of organic compounds [11–13] with their unique physical and physicochemical properties [14]. The clay materials have the specific layered structures and therefore they can easily be exfoliated in aqueous medium to prepare a stable colloidal dispersion [15]. Also it is already reported that clay can efficiently control the aggregation behaviour of various cationic organic dye molecules in different environment [13,16]. Therefore, if two dye

\* Corresponding author.

E-mail addresses: [pkpaul@phys.jdvu.ac.in](mailto:pkpaul@phys.jdvu.ac.in), [pabitra\\_tu@yahoo.co.in](mailto:pabitra_tu@yahoo.co.in)  
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Sammisani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

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63

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## Interpretation of species habitat relationship and animal interaction through remote sensing with reference to spotted deer and langur populations in Kanha National Park, India

Debashis Roy<sup>1\*</sup> and Kamonasish Mistry<sup>2</sup>

*Sammilani Mahavidyalaya, Baghajatin, E.M. By Pass, Kolkata - 94, West Bengal, India.*  
(Assistant Professor in Zoology<sup>1</sup>, Assistant Professor in Geography<sup>2</sup>)

(Received 17 May, 2020; accepted 3 July, 2020)

### ABSTRACT

The Spotted deer (*Axis axis*) and the Langur (*Semnopithecus entellus*) are the two sympatric herbivorous species that live in Kanha National Park of central India. They belong to two different weight categories under family Cervidae and Cercopithecidae. They share habitat, resources and suffer from the same generalist predators. Determining interactions between sympatric Local populations of spotted deer and Langur, in different spatially apart forest sections categorized, grouped and ranked based NDVI values are our prime target. We considered remote sensing technology, field study, NDVI values and location-based photographs to characterize and categorized the forest vegetation. Then the locations of the animals were specified with in NDVI map differentiated into multiple 1x1 sq.km grids and 250 m circular grids. The grid specific data of forest vegetation and respective NDVI values were taken in to consideration for evaluating the species habitat relationships and possible underlying interaction between two sympatric species, spotted deer and langur, under changing environment. Both the species are found to follow dynamic pattern in habitat usages and in interspecific interactions, either by mutual co-existence (Mutualism: +/+) or by competition (Parasitism +/-) as reported by previous researches.

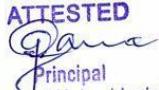
*Key words: Habitat heterogeneity, Remote sensing, NDVI values; Resources, Mutualism.*

### Introduction

Interspecific interactions between two sympatric species are studied for long. The past study mostly concentrated on mammalian populations (Nautiyal & Huffman, 2018; Tsuji et al., 2015) especially between herbivores and primates. Deer of different species across the world were tested while interacting with sympatric primates of different species. In Indian sub-continent, such studies were conducted mainly between spotted deer (*Axis axis*) and langur (*Semnopithecus entellus*). Kanha National Park (lon-

gitude 80° 26' 10.22" E and latitude 22° 12' 52.22" N) of Madhya Pradesh, India is the most explored forest in South-East Asia where behavior of spotted deer and Langur were studied exclusively to understand the ecology and interaction between them. The Kanha national Park is a large heterogeneous forest that composed of dry and wet deciduous Plants (Schaller, 1967). It serves many large mammalian herbivore and omnivore species of which the spotted deer is predominant. Among the primates, the langur is most abundant. Habitat overlapping between these two spe-

\* Corresponding author's email : kamonasish79@gmail.com; debashis675@gmail.com

ATTESTED  
  
Principal  
Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

76 60

Jordan Journal of Mathematics and Statistics (JJMS) 14(2), 2021, pp 197 - 220

## A NEW TYPE OF FUZZY COVERING PROPERTY FOR FUZZY TOPOLOGICAL SPACES

SUMITA DAS(BASU)<sup>(1)</sup>, M. N. MUKHERJEE<sup>(2)</sup> AND PRAKASH MUKHERJEE<sup>(3)</sup>

**ABSTRACT.** In this paper, we introduce and study a new type of fuzzy  $S$ -closedness in a fuzzy topological space with respect to certain fuzzy grill  $\mathcal{G}$  and through some specific  $\alpha$ -shading ( $0 < \alpha < 1$ ), named as fuzzy  $\mathcal{G}_\alpha^S$ -closedness. The work done in this paper aspires to get, in a new perspective, certain analogues of the results and concepts-usually encountered in connection with the study of  $S$ -closedness in topological and fuzzy topological spaces.

### 1. INTRODUCTION AND PRELIMINARIES:

The introductions of fuzzy sets by Zadeh [21] in 1965 and fuzzy topology by Chang [5] in 1968, created a new area for the subsequent rapid development for the extensions of various concepts and their properties from classical set topological case to the wider framework of fuzzy topological space. Among them, an interesting topological covering property named  $S$ -closedness was introduced by Thompson [20] and in its hierarchy, fuzzy  $S$ -closedness was first introduced by Mukherjee and Ghosh [17] in 1989. It was Gantner et al.[8] who designed a totally novel concept of covering named  $\alpha$ -shading ( $\alpha$ -being a member of a designated lattice) and developed a new definition of fuzzy compactness.

On the other hand, observing the importance and wide applicabilities of the idea of grill in set topology, the notion of fuzzy grill was innovated by Azad [1] in 1981.

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*Key words and phrases.* Semi-open  $\alpha$ -shading, proximate  $\mathcal{G}_\alpha$ -shading, fuzzy  $\mathcal{G}_\alpha^S$ -closed, fuzzy  $\mathcal{G}_\alpha$ -compact, fuzzy  $\mathcal{G}_\alpha$ -almost compact.

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Principal  
Samitani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

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63

## The Cultural Politics of “Spring Thunder”: The Naxalbari Movement and the Re-framing of Bengali Culture in the 1960s

Samrat Sengupta, Saikat Maitra

### Abstract

This article tracks the radical turn in Bengali politics and culture and from the late 1960s, ushered in by the ultra-leftist Naxalbari Movement in the eastern Indian state of West Bengal. The movement initiated a search for a Maoist revolutionary praxis that could decisively liberate the dominant Bengali cultural sphere from its moorings in colonial and semi-feudal bourgeois class interests. The counter-hegemonic cultural praxis of the Naxalbari Movement repeatedly evaded its confinement within the diktats of a hardened party line (of the Communist Party of India – Marxist Leninist, which led the movement) but remained rich with multifarious possibilities, openings and narratives. The transgressive vision of this movement led to iconoclastic acts of destroying statues of deified cultural figures, publicly burning canonical books and assaulting higher academic institutions as sites of the propagation of a repressive culture. This article foregrounds the Naxalbari cultural debates along two distinct axes – the received tradition of Bengali culture from the colonial era and the internal schisms among intellectuals and cultural workers sympathetic to the broader objectives of the revolutionary culture articulated through the Naxalbari movement.

**Keywords:** India, Naxalbari, Maoism, West Bengal, politics, Spring Thunder, bhadrolok

### Introduction

This article delineates the radical turn in Bengali cultural productions especially in terms of the co-constitutions of the spheres of the “cultural” and the “political”, which arose in the wake of the Maoist Naxalbari Movement from the late 1960s in the eastern Indian state of West Bengal. While we focus primarily on the cultural debates raging amongst Bengali intellectuals and activists associated with the movement, the political repercussions of Naxalbari, in the period under review, had a far more expansive pan-Indian presence. For instance, Maoist insurrections and their associated socio-cultural imaginaries swept over

Samrat Sengupta, Department of English, Sammilani Mahavidyalaya, Kolkata, India; samrat19802003@yahoo.co.in. Saikat Maitra, Indian Institute of Management, Kolkata, India; saikatmaitro@gmail.com.



ATTESTED  
*Jane*  
 Principal  
 Sammilani Mahavidyalaya  
 E.M. Bypass, Baghajatin  
 Kolkata-700094



# Algae and bacteria consortia for wastewater decontamination and transformation into biodiesel, bioethanol, biohydrogen, biofertilizers and animal feed: a review

Uttpal Anand<sup>1</sup> · Satarupa Dey<sup>2</sup> · Dipannita Parial<sup>3</sup> · Stefania Federici<sup>4,5</sup> · Serena Ducoli<sup>4,5</sup> · Nanthi S. Bolan<sup>6</sup> · Abhijit Dey<sup>7</sup> · Elza Bontempi<sup>4,5</sup>

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## Abstract

Traditional wastewater treatment has been aimed solely at sanitation by removing contaminants, yet actual issues of climate change and depletion of natural resources are calling for methods that both remove contaminants and convert waste into chemicals and fuels. In particular, biological treatments with synergic coupling of microalgae and bacteria appear promising to remove organic, inorganic, and pathogen contaminants and to generate biofuels. Here, we review the use of algae and bacteria in the treatment and valorization of wastewater with focus on cell-to-cell adhesion, wastewater properties, and techniques for algae harvesting and production of biodiesel, bioethanol, biohydrogen, exopolysaccharides, biofertilizers, and animal feeds.

**Keywords** Microalgae · Wastewater treatment and bioremediation · Nutrient removal · Biodiesel and bioethanol production · Biofertilizer production · Emerging contaminants removal

## Introduction

Water is considered the most essential component for all living organisms. Almost 70% of the Earth's surface comprises water, of which nearly 3% accounts for freshwater resources. As freshwater is scarce, sustainable use of water is a pressing need. Recent studies have shown the outbreak of several water-borne diseases among people due to the

consumption of water contaminated with industrial waste and wastewater treatment plants (Hasan et al. 2019; Lin et al. 2022; Ntajal et al. 2022). Various sources of water including municipal, industrial, and agricultural are adding nutrients, toxic metals, colorants, pharmaceutical products, antibiotic residues, pesticides, and inorganic compounds to the water bodies leading to their eutrophication and contamination (Kunhikrishan et al. 2012). The addition of excess nitrogen and phosphorus to wastewater and subsequent eutrophication is considered extremely harmful to aquatic flora and

Uttpal Anand and Satarupa Dey have contributed equally.

✉ Satarupa Dey  
dey1919@gmail.com

✉ Stefania Federici  
stefania.federici@unibs.it

✉ Elza Bontempi  
elza.bontempi@unibs.it

<sup>1</sup> Zuckerberg Institute for Water Research, Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Sede Boqer Campus, 8499000 Midreshet Ben Gurion, Israel

<sup>2</sup> Department of Botany, Shyampur Siddheswari Mahavidyalaya (affiliated to University of Calcutta), Howrah, West Bengal 711312, India

<sup>3</sup> Department of Botany, Sammilani Mahavidyalaya (affiliated to University of Calcutta), Baghajatin, E.M. Bypass, Kolkata, West Bengal 700094, India

<sup>4</sup> Department of Mechanical and Industrial Engineering, University of Brescia, Via Branze 38, 25123 Brescia, Italy

<sup>5</sup> INSTM: Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali, Firenze, Italy

<sup>6</sup> UWA School of Agriculture and Environment and the UWA Institute of Agriculture, The University of Western Australia, Perth, WA 6009, Australia

<sup>7</sup> Department of Life Sciences, Presidency University, 86/1 College Street, Kolkata, West Bengal 700073, India

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ATTESTED  
*Gana*  
Principal  
Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094

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38  
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# Adsorption of 4-Mercapto Pyridine with Gold Nanoparticles Embedded in the Langmuir–Blodgett Film Matrix of Stearic Acid: SERS, XPS Studies Aided by Born–Oppenheimer on the Fly Dynamics, Time–Resolved Wavelet Transform Theory, and DFT

Somsubhra Saha,<sup>||</sup> Bipan Dutta,<sup>||</sup> Manash Ghosh, and Joydeep Chowdhury\*

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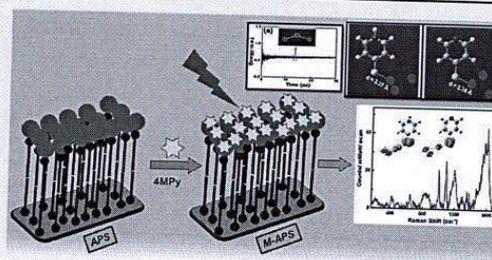
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**ABSTRACT:** This paper reports the adsorptive behavior of the 4-mercaptopyridine (4MPy) molecule soaked in gold nanoparticles (AuNPs) that remain embedded in the bilayer Langmuir–Blodgett (LB) film matrix of stearic acid (SA) for various soaking times (STs). The as-fabricated substrate proved to be an efficient SERS sensing platform that can sense the analyte 4MPy molecules at trace concentrations of  $\sim 1.0 \times 10^{-9}$  M. The XPS study not only reveals the adsorption of 4MPy molecules with AuNPs via a sulfur atom but also suggests partial degradation of the analyte molecule upon adsorption. This observation is further substantiated from the SERS spectral profile, which shows unusual broadening of the enhanced Raman bands of the molecule at higher STs. The experimental observations are supported by Born–Oppenheimer



on-the-fly molecular dynamics (BO-OF-MD), time-resolved wavelet transform theory (WT), and the DFT calculations based on adcluster models. Selective enhancements of Raman bands in the SERS spectra further suggest the involvement of charge transfer (CT) interaction to the overall enhancements of Raman bands of the analyte molecule. The molecule  $\rightarrow$  CT contribution has been estimated from electron density difference calculations and the corresponding CT distance; the amount of CT is also envisaged.

## 1. INTRODUCTION

Surface-enhanced Raman scattering (SERS) spectroscopy<sup>1</sup> has opened up new horizons not only in the offing of analytical sciences but also in elucidating the physics and chemistry of the surfaces.<sup>2–7</sup> Although the underlying reason behind colossal enhancements in the Raman signals has now been unanimously acclaimed to originate broadly from electromagnetic (EM) and charge transfer (CT) mechanisms, there however has been renewed interest in fabricating new SERS active substrates and understanding their adsorptive behaviors with the aid of improved adatom models.<sup>8–11</sup> While fabrications of new SERS active substrates that offer promising applications in the real-world diagnostics and in forensic sciences have gained significant attention from material scientists these days,<sup>12–15</sup> improved ad-cluster molecule–metal ( $M_n$ ,  $n = 1$  to 20) models from quantum chemical calculations proved to be effective in understanding their adsorptive behaviors.<sup>16–21</sup>

Considering the above issues, the present paper reports facile fabrication of a SERS active substrate through integration of self-assembly and Langmuir–Blodgett (LB) deposition techniques. Efficacy of the as-fabricated substrate has been tested from the SERS spectra of the analyte 4-mercaptopyr-

idine (4MPy) molecule. The adsorptive site of the analyte molecule with the substrate has been investigated in detail from X-ray photoelectron spectroscopy (XPS) studies. The experimental observations are aided by Born–Oppenheimer on-the-fly molecular dynamics (BO-OF-MD), time-resolved wavelet transform theory, and density functional theory (DFT) calculations based on analyte molecule–metal adcluster models. To the best of our knowledge, this paper may be considered the first ever report where the most probable molecule–adcluster model has been proposed from BO-OF-MD followed by DFT calculations. The CT contribution to the overall enhancement of the SERS spectra of the 4MPy molecule has also been envisaged from electron density difference (EDD) studies.

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44  
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## Effect of silver nanoparticles on nitrogen-cycling bacteria in constructed wetlands

Monolina Sarkar<sup>1</sup>

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### Abstract

Silver nanoparticles (AgNPs) are one of the most popular engineered nanomaterials (ENMs) because of their anti-microbial properties. In wastewater treatment ecosystems, ENMs can be removed by plant uptake or adsorption on biofilms. However, AgNPs can inhibit the activities of plants and microorganisms. This review outlines the effects of AgNPs on nitrogen-cycling bacteria in constructed wetlands (CWs). Environmental conditions like organic matter, pH, ionic strength of soil along with the size, concentration, surface coating, speciation, and aggregation of AgNPs influence the toxicity. Bacterial activity is hampered by disruption of the cell membrane and extracellular polymers, reactive oxygen species (ROS) imbalance, DNA damage, inhibition of gene expression, protein functions, and energy production. Compared to heterotrophic bacteria, generally, nitrifying bacteria are more sensitive to AgNPs. Bacterial inhibition leads to a significant decrease in community diversity and reduction in nitrogen removal efficiency (NRE). Recovery of NRE is correlated with the resistance and functional redundancy of the community. Exposure to sublethal AgNP concentrations can upregulate nitrogen-cycling genes. The hormetic response and bacterial resilience are more evident in communities with high diversity. Plants enrich the diversity of nitrogen-cycling bacteria in planted CWs in the presence of AgNPs. Compared to unplanted CWs, the planted wetlands are resistant to AgNPs and consequently exhibit a better NRE after long-term exposure. Future endeavors to analyze the influence of AgNPs should be preceded by a long-term assessment of the complex interactions in actual treatment systems that are often overlooked in studies using synthetic wastewater.

**Keywords** Anammox · Bacterial community diversity · Denitrification · Ecotoxicology · Microbial ecology · Nitrification

### Introduction

Over the last few years, the systematically designed nanoscale materials or engineered nanomaterials (ENMs) have been used for various purposes. This wide application is due to their unique attributes such as small size (1–100 nm), large surface area to volume ratio, high reactivity, high carrier capacity, high surface energy, quantum confinement, and easy variation of surface properties [1]. Silver nanoparticles (AgNPs) are one of the most frequently used ENMs. Because of their anti-microbial characteristics, they are widely used in several industries including food packaging, textile, medical devices, and health care [2, 3]. Furthermore,

they have been used in catalysis, electronics, and as biosensors [4]. In the agriculture sector, AgNPs can function as plant growth stimulators, bactericides, fungicides, and insecticides [5–7]. The global manufacture of AgNPs has been projected to reach almost 800 tons by the year 2025 [8]. With increasing usage, AgNPs may be released into the environment by sewage discharge and surface runoff [9, 10]. As the last barrier in eliminating contaminants, constructed wetlands (CWs) are a sustainable, inexpensive technology for removing pollutants from wastewater. AgNP attachment to sludge biomass is one of the important processes promoting their removal [11]. As ENMs, including AgNPs from runoffs, may eventually build up in CWs, they may affect the bacterial community and consequently the bacteria-mediated nutrient removal [12–18].

CWs are dependent on the bacterial community structure for performing nitrogen removal [19]. In the nitrification–denitrification (NDN) process, chemoautotrophic nitrifying bacteria are one of the major contributors

✉ Monolina Sarkar  
monolinasarkar1@gmail.com

<sup>1</sup> Department of Botany, Sammilani Mahavidyalaya, Baghajatin, E.M. Bypass, Kolkata, West Bengal 700094, India



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Special Issue Article

## Nod factor-independent 'crack-entry' symbiosis in dalbergoid legume *Arachis hypogaea*

Sohini Guha ✉, Firoz Molla, Monolina Sarkar, Fernando Ibañez, Adriana Fabra, Maitrayee DasGupta ✉

First published: 07 January 2022 | <https://doi.org/10.1111/1462-2920.15888> | Citations: 7



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### Summary

Dalbergoids are typified by crack-entry symbiosis which is evidenced to be Nod Factor (NF)-independent in several *Aeschynomene* legumes. Natural symbionts of the dalbergoid legume *Arachis hypogaea* are always NF-producing, prompting us to check whether symbiosis in this legume could also be NF-independent. For this, we followed the symbiosis with two NF-containing bradyrhizobial strains – SEMIA6144, a natural symbiont of *Arachis* and ORS285, a versatile nodulator of *Aeschynomene* legumes, along with their corresponding nodulation (*nod*) mutants. Additionally, we investigated NF-deficient bradyrhizobia like BTA11, a natural symbiont of *Aeschynomene indica* and the WBOS strains that were natural endophytes of *Oryza sativa*, collected from an *Arachis-Oryza* intercropped field. While SEMIA6144Δ*nodC* was non-nodulating, both ORS285 and ORS285Δ*nodB* could induce functional nodulation, although with lower

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Kolkata-700094

efficiency than SEMIA6144. On the other hand, all the NF-deficient strains – BTAi1, WBOS2 and WBOS4 showed comparable nodulation with ORS285 indicating *Arachis* to harbour an NF-independent mechanism of symbiosis. Intriguingly, symbiosis in *Arachis*, irrespective of whether it was NF-dependent or independent, was always associated with the curling or branching of the rosette root hairs at the lateral root bases. Thus, despite being predominantly described as an NF-dependent legume, *Arachis* does retain a vestigial, less-efficient form of NF-independent symbiosis.

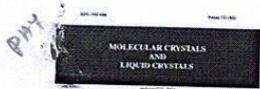
### Supporting Information

Filename	Description
emi15888-sup-0001-Figures1.jpg 4.1 MB	<p><b>Fig. S1.</b> Labelling of <i>Bradyrhizobium</i> via Tn7 transposition (A) Map representing the sfgFP and mCherry cassettes along with the spectinomycin encoding gene <i>aad9</i>, bounded by Tn7L and Tn7R which indicate the left and right extremities of the insertion clusters, marked with a crimson line, integrated downstream to the <i>gImS</i> gene of bradyrhizobial genomes. The black arrows marked '<i>gImS<sub>down</sub></i>' and '<i>aad9<sub>rev</sub></i>' represent the primer positions used for identifying the point of Tn7 insertion. (B) Comparative DNA gel images showing the absence and presence of a 1.5 kb amplicon corresponding to the PCR against the primer pair <i>gImS<sub>down</sub>-aad9<sub>rev</sub></i> in the unlabelled and labelled <i>Bradyrhizobium</i>. Positive PCR indicates the integration of the Tn7 cluster within the selected strains. (C) Nucleotide sequence alignment showing the region downstream to the <i>gImS</i> gene (shaded in ash) of the labelled <i>Bradyrhizobium</i> strains. The Tn7 point of insertion has been marked with a</p>

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## Interaction of hectorite clay with a phospholipid monolayer at air-saline interface in presence of a fluorescent dye

Tanmoy Singha, Ujjal Saren, Pradip Maiti, Utsav Chakraborty, Alapan Pal & Pabitra Kumar Paul

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## Interaction of hectorite clay with a phospholipid monolayer at air-saline interface in presence of a fluorescent dye

Tanmoy Singha, Ujjal Saren, Pradip Maiti, Utsav Chakraborty, Alapan Pal, and Pabitra Kumar Paul 

Department of Physics, Jadavpur University, Kolkata, India

### ABSTRACT

The effect of hectorite clay on the monolayer of 1, 2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) at air-saline interface in presence of fluorescent dye acridine orange (AO) is studied. Surface pressure-area isotherm and compressibility studies reveal the phase behavior and rheological properties of DPPC monolayer. Formation of DPPC/clay complex and their aggregation during monolayer compression partially remove DPPC molecules from the interface. UV-vis absorption and fluorescence emission techniques confirm the aggregation of AO in DPPC/clay/AO hybrid Langmuir-Blodgett film. As phospholipids act as lung surfactants, this model study has implication of realizing the detrimental effects of clay on phospholipids during alveolar surface compression while breathing.

### KEYWORDS

acridine orange; bio-membrane; DPPC; hectorite; isotherm; Langmuir-Blodgett

### 1. Introduction

Amphiphilic molecules show interesting surface-active properties and form insoluble monolayer when they are spread at the air water interface. This is known as Langmuir monolayer. Langmuir monolayer has been widely investigated by the analysis of surface pressure versus area per molecule ( $\pi$ -A) isotherm which gives a well-defined, two dimensional media where molecular orientation, packing density, surface tension and phase behavior can be controlled by changing various parameters. Langmuir monolayer is very useful to precisely understand the molecular level interactions especially for various bio-molecular interface such as membranes [1-3]. Nowadays there is big concern about some harmful effects of inorganic layered nanomaterials such as clay minerals on biologicals membranes [4]. Phospholipids are well known as the primary component for bio-membrane and therefore the study of interactions of nanoclay with phospholipid membrane is of major importance. Phospholipid monolayer are used as a fundamental ex-vivo model of a cell membrane but they are also used to explore the interfacial properties of lung (or pulmonary) surfactant (LS) [5]. Respiratory symptoms and undesired health effects are caused by inhalation of dust particles formed from the mineral materials present in the environment. Another complex problem in our health is occurred due to aerosol deposition in our respiratory system [6,7]. As the Langmuir monolayer

CONTACT Pabitra Kumar Paul  pabitra\_tu@yahoo.co.in; pabitrak.pal@jadavpuruniversity.in  Department of Physics, Jadavpur University, Jadavpur, Kolkata, 700032, India  
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E.M. Bypass, Baghajatin  
Kolkata-700094

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# Comparative and Selective Interaction of Amino Acid D-Cysteine with Colloidal Gold Nanoparticles in the Presence of a Fluorescent Probe in Aqueous Medium

Pradip Maiti, Ujjal Saren, Utsav Chakraborty, Tanmoy Singha, Sharmistha Paul, and Pabitra Kumar Paul\*

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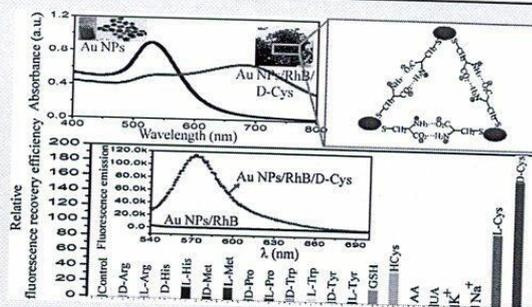
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**ABSTRACT:** In this communication, we report the comparative and selective interaction of amino acid D-cysteine (D-Cys) with citrate capped gold nanoparticles (Au NPs) in the presence of a fluorescent dye, rhodamine B (RhB), in aqueous solution. Au NPs of size 27.5 nm could almost fully quench the steady-state fluorescence emission of RhB at their optimum concentrations in the mixed solution. The interactions of D-Cys, L-Cys, all other relevant D- and L-amino acids, neurotransmitters, and other relevant biological compounds with the Au NPs/RhB mixed solution have been explored by monitoring the fluorescence recovery efficiencies from the almost fully quenched state of RhB fluorescence via a simple steady-state spectrofluorometric method. The higher fluorescence recovery for the interaction of D-Cys with the Au NPs/RhB mixed system is accompanied by a distinct color change (red-wine to bluish-black) of the assay medium after the reaction compared to that of all other interfering compounds considered in this work. The sensitivity of this fluorometric response lies in a broad linear range of concentrations of D-Cys and the limit of detection (LOD) is found to be 4.2 nM, which is low compared to many other methods available in the literature. The different degrees of interaction of D-Cys and L-Cys with the Au NPs/RhB mixed sample have been further explored by circular dichroism (CD) spectroscopy and Fourier transform infrared (FTIR) spectroscopy. The selective interaction of D-Cys with the proposed Au NPs/RhB mixed system is also found to be correlated with interparticle cross-linking and aggregations of nanoparticles by the analysis of  $\zeta$  potential and dynamic light scattering (DLS) study, transmission electron microscopy (TEM), atomic force microscopy (AFM), UV-vis absorption spectroscopy etc. The proposed interaction mechanism is further studied with a normal human urine sample to elucidate that the optimized combination of Au NPs and RhB may be realized as an efficient platform for detection of the amino acid D-Cys in a real biosample via a simple fluorometric approach.



## 1. INTRODUCTION

The fundamental part of antibodies, signaling molecules, enzymes, hormones, receptors, and protein structures present in all living organisms is amino acids. They also act as biochemical rulers in the neurotransmission.<sup>1,2</sup> All of the amino acids present in the nature exist mainly in two forms: dextrorotatory (D) and levorotatory (L) enantiomers. On the basis of the protein-creating efficiency, there are in total 20 amino acids that have been reported. Previously, it was presumed that only L-amino acids were necessary in mammals, including humans, in the formation of components for proteins and peptides. However, various sensitive and selective analytical approaches developed for detecting chiral amino acids<sup>3,4</sup> suggested that diverse D-amino acids are also present in mammalian tissues. Different studies have been performed to explore the physiological functions of D-amino acids. The physiological and the biochemical activities of different D-

amino acids such as D-cysteine (D-Cys), D-aspartate (D-Asp), D-alanine (D-Alan), D-serine (D-Ser) etc. in our nerve cells, skin, arterial walls, bones, other tissues, and body fluids, including amniotic fluid, urine, blood plasma, cerebrospinal fluid (CSF), saliva etc., have been systematically studied by various researchers in the last several years.<sup>5,6</sup>

The semi-essential, proteinogenic amino acid cysteine (C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S) (abbreviated as Cys) contains thiol (–SH), amine (–NH<sub>2</sub>), and carboxylic (–COOH) functional groups.

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*Pabitra Kumar Paul*  
Principal  
Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094  
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## Geographical Appraisal of COVID-19 in West Bengal, India

Biplab Biswas · Rabindranath Roy · Tanusri Roy · Sumanta Chowdhury ·  
Asish Dhara · Kamonasish Mistry

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**Abstract** Study shows that COVID-19 cases, deaths and recoveries vary in macro level. Geographical phenomena may act as potential controlling factor. The present paper investigates spatial pattern of COVID-19 cases and deaths in West Bengal (WB), India and assumes Kolkata is the source region of this disease in WB. Thematic maps on COVID related issues are prepared with the help of QGIS 3.10 software. As on 15th January 2021, WB has 564032 number of COVID-19 cases which is 0.618% to the total population of the state. However, the COVID-19 case for India is 0.843% and for world is 1.341% to its total population. Lorenz Curve shows skewed

distribution of the COVID-19 cases in WB. 17 (90%) districts hold 84.11% of the total population and carry 56.30% of the total COVID-19 cases. However, the remaining two districts—Kolkata and North 24 Parganas—hold remaining 43.70% COVID-19 cases. Correlation coefficient with COVID-19 cases and Population Density, Urban Population and Concrete Roof of their house are significant at 1% level of significance.

**Keywords** COVID-19 · West bengal · Geographical factor · Urbanization · Population density · Nonworking population · Forest

B. Biswas (✉) · T. Roy · S. Chowdhury ·  
A. Dhara · K. Mistry  
Department of Geography, The University of Burdwan,  
Purba Bardhaman, West Bengal 703104, India  
e-mail: bbiswas@geo.buruniv.ac.in

T. Roy  
e-mail: roytanusri.26@gmail.com

S. Chowdhury  
e-mail: sumantachowdhury421@gmail.com

A. Dhara  
e-mail: dharaasish91@gmail.com

K. Mistry  
e-mail: kamonasish79@gmail.com

R. Roy  
Department of Community Medicine, Burdwan Medical  
College and Hospital, Burdwan 713104, India  
e-mail: rabinroynew@gmail.com

### Introduction

Novel coronavirus (2019-nCov) is wreaking havoc worldwide. As on 15th January 2021, the virus-related disease COVID-19, killed about 2,009,092 human lives, spreading over 273 countries. However, in the macro (even in micro) level, there are spatial variations on its cases and deaths. Data from published epidemiology and virology studies provide evidence of 2019-nCov transmission from infected peoples to others who are in direct contact or close contact through respiratory droplets, or by contact with contaminated objects and surfaces. A recent study shows that the novel coronavirus disease can spread

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## A novel carbazole-benzothiazole-based chemodosimeter for the chromogenic and fluorogenic recognition of $\text{CN}^-$ †

Atanu Maji, Amitav Biswas, Akash Das, Saswati Gharami, Krishnendu Aich and Tapan K. Mondal\*

A novel colorimetric and fluorescent sensing probe, (*E*)-3-(4-(9H-carbazol-9-yl)phenyl)-2-(benzo[d]thiazol-2-yl)acrylonitrile (CBTA), was synthesized and characterized by spectroscopic techniques. CBTA displayed "turn off" fluorescence in the presence of cyanide with a higher selectivity than that of others anions such as  $\text{Br}^-$ ,  $\text{Cl}^-$ ,  $\text{I}^-$ ,  $\text{NO}_3^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{SCN}^-$ ,  $\text{CO}_3^{2-}$ ,  $\text{N}_3^-$ ,  $\text{OH}^-$ ,  $\text{HCO}_3^-$ ,  $\text{H}_2\text{PO}_4^-$ ,  $\text{HPO}_4^{2-}$ ,  $\text{F}^-$ ,  $\text{ACO}^-$ , and  $\text{PO}_4^{3-}$  in a DMSO:H<sub>2</sub>O medium (40:60, v/v, HEPES buffer, pH = 7.2). The "turn off" fluorescence response mechanism can be attributed to the intra-molecular charge transfer (ICT) process, which is blocked by the nucleophilic attack of cyanide ions at the cyano vinyl group of the probe. The LOD was found to be  $3.57 \times 10^{-8}$  M. The interaction involved behind the sensing of cyanide was investigated by Job's plot analysis, <sup>1</sup>H-NMR, and mass spectroscopic studies. DFT and TDDFT were also employed to verify the experimental outcomes. Moreover, the test strip experiment provides a wide application prospect of the receptor for detecting poisonous cyanide in the environment and biological system.

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### Introduction

The development of a new molecular probe for the detection of anions is of great interest because of their vital roles in a wide range of medicines, catalysis, life science, and environment.<sup>1</sup> Additionally, food safety issues and water pollution by poisonous anions have drawn attention with the development of science and technology nowadays.<sup>2–6</sup> Cyanide is one of the most well-known toxic anions, even at a lower concentration, which can be lethal to human beings, animals, and environment. Cyanide is currently extensively used in many industrial processes such as electroplating, petrochemicals, photography, steel production, gold mining, metallurgy, and the synthesis of resin and fibre due to its critical role in multi-functional reactions.<sup>7</sup> World Health Organization (WHO) stipulates that the permissible acceptable concentration of cyanide in drinking water is  $1.9 \times 10^{-6}$  mol L<sup>-1</sup>.<sup>8</sup> By the way, cyanide is present in some insects, fruits, seeds, and roots where it is released through the hydrolysis process of cyanogenic glycosides.<sup>9–14</sup> Cyanide binds to the iron ion in cytochrome *c* oxidase, blocks the electron transport in metabolism, and inhibits the

production of ATP in cells, making the biological system inefficient to provide sufficient energy to the heart, central nervous system and other vital organs ultimately.<sup>15,16</sup> Considering the above-mentioned fact, the development of simple, efficient and rapid detection tools with high selectivity and sensitivity towards cyanide is an ongoing hot topic to prevent the harmful effect in the human body from contaminated food and environment.

To date, fluorescent molecular probes capable of detecting  $\text{CN}^-$  have been reported based on fluorescence resonance energy transfer (FRET),<sup>17–19</sup> intra-molecular charge transfer (ICT),<sup>20,21</sup> twisted intra-molecular charge transfer (TICT),<sup>22</sup> excited state intra-molecular proton transfer (ESIPT),<sup>23,24</sup> and photo-induced electron transfer (PET).<sup>25,26</sup> Recently, several groups have reported detection methods by utilizing the nucleophilic addition reaction of cyanide directly involved in the development of covalent bond formation and showed anti-interference ability and high selectivity.<sup>27–38</sup> Compared with the traditional sophisticated analytical tools such as spectrophotometry, voltammetry, chromatography, and potentiometric methods, optical molecular probes based on colorimetric and fluorometric responses towards  $\text{CN}^-$  are of great preference in virtue of their convenience, simplicity, tenability, low cost, high selectivity and rapid response.<sup>39</sup> Particularly, a naked-eye optical sensor is very much impressive. Since the Tang *et al.* discovery of the AIE phenomenon in 2001, several research groups have been published a growing number of AIE active

Department of Chemistry, Jadavpur University, Kolkata-700032, India.

E-mail: [tapank.mondal@jadavpuruniversity.in](mailto:tapank.mondal@jadavpuruniversity.in)

† Electronic supplementary information (ESI) available: NMR and MS of all new compounds, limit of detection determination, quantum yield calculation. See DOI: <https://doi.org/10.1039/d3nj01157g>

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## Enhancement of Fluorescence Mediated by Silver Nanoparticles: Implications for Cell Imaging

Pradip Maiti, Swarupa Sarkar, Tanmoy Singha, Sannak Dutta Roy, Mrityunjoy Mahato, Parimal Karmakar, Sharmistha Paul, and Pabitra Kumar Paul\*

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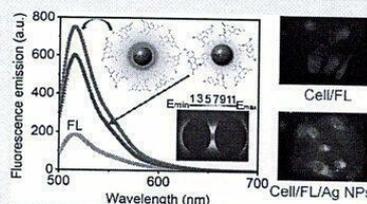
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**ABSTRACT:** In this study, we report the surface enhanced fluorescence (SEF) of a biologically important organic dye, fluorescein (FL), by silver nanoparticles (Ag NPs) in an aqueous medium and its implications for human cell imaging. The synthesized Ag NPs were characterized by dynamic light scattering (DLS), zeta potential, transmission electron microscopy (TEM), and UV–vis absorption spectroscopic studies. The interaction and aggregation of FL dye with Ag NPs and a cationic surfactant, namely, cetyltrimethylammonium bromide (CTAB), were explored by UV–vis absorption and steady-state and time-resolved fluorescence spectroscopic methods. The distance-dependent fluorescence enhancement of FL due to Ag NPs in the solution was also theoretically correlated by three-dimensional finite-difference time-domain (3D-FDTD) simulation. The plasmonic coupling between neighboring NPs facilitated the augmentation of the local electric field, thereby producing various “hotspots” that influence the overall fluorescence of the emitter. J-type aggregates of FL in the presence of the CTAB micelles and Ag NP mixed solution were confirmed by electronic spectroscopy. The density functional theoretical (DFT) study revealed the electronic energy levels associated with different forms of FL dye in the aqueous solution. Most interestingly, the Ag NP/FL mixed system used in fluorescence imaging of human lung fibroblast cells (WI 38 cell line) showed a significantly stronger green fluorescence signal compared to that of FL after an incubation period of only 3 h. This study confirms that the Ag NP mediated SEF phenomenon of the FL dye is also manifested in the intracellular medium of human cells giving a brighter and more intense fluorescence image. The cell viability test after exposure to the Ag NP/FL mixed system was confirmed by the MTT assay method. The proposed study may have an implication as an alternate approach for human cell imaging with higher resolution and more contrast.



### INTRODUCTION

A wide range of biomedical applications have been developed and commercially available with the advancement of fluorescence emission spectroscopic techniques, synthesis of a variety of new fluorescent compounds, as well as modern device sophistication. The synthesis of new organic and inorganic probe materials with unique physical and physicochemical properties has spurred the systematic investigation of protein localization and biological function of living cells.<sup>1,2</sup> Cellular imaging by the fluorescence technique is an excellent analytical approach that has revolutionized the molecular cell biology and related fields through the assessment or identification of the dynamical behavior of intra- or extracellular components of a variety of living cells in real time, i.e., by fluorescence imaging microscopy.

Fluorescence imaging microscopy is used in many biological assays because of its potentially high sensitivity, selectivity, and ease of use to understand the underlying causes of various diseases at the cellular and molecular level with very low invasiveness and insensitivity toward magnetic and electric signals.<sup>3,4</sup> Although fluorescence imaging microscopy has a long scientific history, this technique itself faces difficulties in

case of fluorophores with low intrinsic light emission, low photostability, and photobleaching<sup>5</sup> as this method essentially demands fluorophores such as organic dyes, quantum dots, etc., with distinct spectral and photophysical properties. Many traditional organic fluorescent dyes are being used as probes in conventional fluorescence microscopy, but, their performance is still limited because of the low spatial and temporal resolution as well as the interference by the background autofluorescence from the cellular environments.<sup>6,7</sup> With the recent advancement of scientific research in the microscopic level, it is therefore very important to improve the performance and sensitivity of such fluorescence-based imaging method by enhancing the intrinsic fluorescence emission of the probes. In view of the performance of various fluorescence-based detection methods, plasmonic metal nanostructures such as

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46  
93



# Light-responsive biodegradation of wastewater pollutants: New developments and potential perspectives

Monolina Sarkar

Department of Botany, Sammilani Mahavidyalaya, Baghajatin, E.M. Bypass, Kolkata, West Bengal 700094, India

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## ABSTRACT

The existence of micropollutants in wastewater is one of the most challenging environmental issues in the world today. Due to their high stability and resistance to physicochemical and biological degradation, pollutants like hormonally active substances, pesticides, industrial chemicals, pharmaceuticals, personal care products, doping substances, and narcotics among others are difficult to remove in wastewater treatment plants (WWTPs). A potential technology for treating pollutants is photocatalytic biodegradation. The advancements in light-responsive biodegradation technologies—namely, intimately coupled photocatalysis and biodegradation (ICPB), microbial fuel cells (MFCs), and photobiocatalysis are highlighted in this work. The article identifies opportunities for refining current methodologies. It aims to provide a perspective for future research devoted to assessing and improving pollutant removal.

## 1. Introduction

The increasing contamination of aquatic environments with recalcitrant contaminants like pharmaceutically active compounds, personal care products, industrial chemicals, polycyclic aromatic hydrocarbons, illicit drugs, pesticides, herbicides, and surfactants, has become a new challenge to global water quality. It is difficult to remove these pollutants from wastewater treatment plants (WWTPs). Prolonged and uncontrolled contact with these micropollutants could contaminate surface and groundwater, wreaking havoc on ecosystems and human health. Biocatalysts or enzymes have the potential to degrade environmental pollutants with high substrate specificity and selectivity under mild conditions. However, their large-scale usage is limited by the high expenses of purification and challenges with recycling and renaturation under practical conditions. Photocatalytic processes cannot treat insufficiently transparent water (Al-Nuaim et al., 2022; Deng et al., 2021; Zhang et al., 2021). Also, incomplete photocatalytic reaction products can be toxic, and mineralization can be expensive. Coupling photocatalysis with biotransformation presents an efficient methodology for the economic and sustainable degradation of recalcitrant pollutants (Özgen et al., 2021; Rittmann, 2018; Zhang et al., 2021). These disadvantages motivate the development of photobiocatalytic systems that combine photocatalytic systems with biocatalytic reactions (Harrison et al., 2022; Maciá-Agulló et al., 2015; Schermund et al., 2019). They combine new reactivity, high enantioselectivity, and better yields with simple and sustainable syntheses as well as recyclability. Till date, only a few known enzymatic reactions require light, and only a selected few exhibit a light-driven promiscuous activity. In most cases, light either provides the co-

substrate or cofactor in a suitable redox state for the biotransformation. Other techniques have combined, light-induced chemical reactions with a biocatalytic step, or light-induced biocatalytic reactions with chemical reactions in a linear cascade. This work provides an overview of the approaches that use light for the biodegradation of wastewater pollutants, namely Intimate Coupling of Photocatalysis with Biodegradation (ICPB), Photo Microbial Fuel Cells (PMFCs), and photobiocatalysts.

Under optimal light intensity, the degradation of recalcitrant organic pollutants can be catalyzed by Intimate Coupling of Photocatalysis with Biodegradation (ICPB) (Liu et al., 2022; Zuo et al., 2021). The protected biofilm harbors a substantial capacity to degrade pollutants and lower the levels of chemical oxygen demand (COD) or dissolved organic carbon (DOC). The macroporous substratum, which anchors the photocatalyst on its exterior shelters the biofilm in its interior from Ultraviolet (UV) light and free radicals. The recalcitrant contaminants transformed by photocatalysis are degraded by the bacterial biofilm. Several recalcitrant contaminants, like phenol (Ma et al., 2015; Zhou et al., 2015), pyridine (Shi et al., 2020), phenanthrene (PHE) (Cai et al., 2019), and tetracycline hydrochloride (TCH) (Xiong et al., 2017) have been proven to be effectively degraded by the ICPB system. Considering that most microbes cannot bear UV light irradiation, visible light has been used to induce Intimate coupling of visible light-induced photocatalysis and biodegradation (VPCB) to treat pollutants (Yu et al., 2020; Zhou et al., 2015). A significantly higher removal efficiency of organic pollutants can be achieved in the VPCB than that induced by UV lights. The enhanced activity is attributed to visible light irradiation and enhanced extracellular polymeric substance secretion that protects the microbial communities in the carriers. The VPCB method also has a better potential energy-saving capability.

E-mail address: [monolinasarkar1@gmail.com](mailto:monolinasarkar1@gmail.com)

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ATTESTED

*Jana*  
Principal

Sammilani Mahavidyalaya  
E.M. Bypass, Baghajatin  
Kolkata-700094