

*List of Academic Publications,  
Conferences and Symposiums Attended*

LIST OF PUBLICATIONS

- [1] Das, D.; Dutta, S.; Dowerah, D. and Deka, R.C. Unveiling the Role of Hydrogen Bonding and g-Tensor in the Interaction of Ru-Bis-DMSO with Amino Acid Residue and Human Serum Albumin. *The Journal of Physical Chemistry B*, 124(30): 6459-6474, 2020.
- [2] Sarma, P.J.; Dowerah, D.; Gour, N.K.; Logsdail, A.J.; Catlow, C.R.A. and Deka, R.C., Tuning the transition barrier of H<sub>2</sub> dissociation in the hydrogenation of CO<sub>2</sub> to formic acid on Ti-doped Sn<sub>2</sub>O<sub>4</sub> clusters. *Physical Chemistry Chemical Physics*, 23(1): 204-210, 2021.
- [3] Uppuladinne, M.V.; Dowerah, D.; Sonavane, U.B.; Ray, S.K.; Deka, R.C. and Joshi, R.R. Structural insight into locked nucleic acid based novel antisense modifications: A DFT calculations at monomer and MD simulations at oligomer level. *Journal of Molecular Graphics and Modelling*, 107: 107945, 2021.
- [4] Biswakarma, N.; Dowerah, D.; Baruah, S.D.; Sarma, P.J.; Gour, N.K. and Deka, R.C., Catalytic oxidation of NO to NO<sub>2</sub> on pure and doped Au<sub>n</sub>Pt<sub>3-n</sub> (n= 0–3) clusters: A DFT perspective. *Molecular Catalysis*, 515: 111910, 2021.
- [5] Devi, Y.D.; Goswami, H.B.; Konwar, S.; Doley, C.; Dolley, A.; Devi, A.; Chongtham, C.; Dowerah, D.; Biswa, V.; Jamir, L. and Kumar, A., Immunoinformatics mapping of potential epitopes in SARS-CoV-2 structural proteins. *PloS one*, 16(11): 0258645, 2021.
- [6] Talukdar, H.; Gogoi, S.R.; Sultana, S.Y.; Begum, R.; Dowerah, D.; Sarma, B. and Islam, N.S., Oxido-and Mixed-Ligand Peroxido Complexes of Niobium (V) as Potent Phosphatase Inhibitors and Efficient Catalysts for Eco-Friendly Styrene Epoxidation. *Dalton Transactions*, 52(29): 10165-10182, 2023.
- [7] Kakati, U.P.; Dowerah, D.; Deka, R.C.; Gour, N.K. and Paul, S. Tropospheric Oxidation of 1, 1, 2, 3-Tetrafluoropropene (CF<sub>2</sub>=CF-CH<sub>2</sub>F) Initiated by ·OH Radical and Aerial Degradation of Its Product Radicals. *ACS Earth Space Chemistry*, 7(2): 501-514, 2023.
- [8] Churi, P.P.; Biswakarma, N.; Dowerah, D.; Neog, S.; Sarma, P.J.; Gour, N.K. and Deka, R.C. Structure and Stability of (CeO<sub>2</sub>)<sub>n</sub><sup>0,+1</sup> (n=1-3) Clusters towards the Adsorption and Co-adsorption of CO and H<sub>2</sub>O from DFT Study. *Chemical Physics Impact*, 6: 100125, 2023.

- [9] Dowerah, D.; VN Uppuladinne, M.; Sarma, P.J.; Biswakarma, N.; Sonavane, U.B.; Joshi, R.R.; Ray, S.K.; Namsa, N.D. and Deka, R.C. Design of LNA analogues using a combined density functional theory and molecular dynamics approach for RNA therapeutics. *ACS omega*, 8(25): 22382-22405, 2023.
- [10] Dutta, P., Biswakarma, N., Dowerah, D., Neog, S., Islam, S., Sarma, S., ... and Deka, R. C. Partial Oxidation of Methane to Methanol by Using Molecular O<sub>2</sub> on Pd<sub>2</sub><sup>+</sup> Catalyst: An Insight from Theory. *Chemistry Select*, 8(33): e202301920, 2023.
- [11] Neog, S., Dowerah, D., Biswakarma, N., Dutta, P., Churi, P. P., Sarma, P. J., ... and Deka, R. C. (2023). Reaction Mechanism and Kinetics for the Selective Hydrogenation of Carbon Dioxide to Formic Acid and Methanol over the [Cu<sub>2</sub>]<sup>0,+1</sup> Dimer. *The Journal of Physical Chemistry A*, 127(41): 8508-8529, 2023.
- [12] Sarma, S., Gour, N. K., Dowerah, D., Begum, S. S., and Deka, R. C. Binding patterns of derivatives of fisetin and chrysin to the enzyme complex cyclin-dependent kinase 6/cyclin D. *Theoretical Chemistry Accounts*, 142(11): 116, 2023.
- [13] Sarma, P. J., Neog, S., Biswakarma, N., Dowerah, D., Dutta, P., Das, T., ... and Deka, R. C. Tuning the Reaction Mechanism toward Selective Hydrogenation of CO<sub>2</sub> to Formic Acid on a Sn<sub>10</sub>O<sub>20</sub> Cluster. *Industrial & Engineering Chemistry Research*, 62(51): 21967-21976, 2023.
- [14] Sarma, S., Dowerah, D., Basumatary, M., Phonglo, A., and Deka, R. C. Inhibitory potential of furanocoumarins against cyclin dependent kinase 4 using integrated docking, molecular dynamics and ONIOM methods. *Journal of Biomolecular Structure and Dynamics*, 1-30, 2023.
- [15] Kakati, U. P., Dowerah, D., Deka, R., Gour, N. K., and Paul, S. Oxidation Pathways and Kinetics of 1,1,2,3-Tetrafluoropropene (CF<sub>2</sub>=CF-CH<sub>2</sub>F) Reaction with Cl-atoms and Subsequent Aerial Degradation of its Product Radicals in Presence of NO. *Environmental Science: Processes & Impacts*, 2024.
- [16] Dolley, A., Goswami, H. B., Dowerah, D., Dey, U., Kumar, A., Hmuaka, V., ... and Namsa, N. D. Reverse vaccinology and immunoinformatics approach to design a chimeric epitope vaccine against *Orientia tsutsugamushi*. *Heliyon*, 10(1), 2023.
- [17] Gogoi, G.; Joarder, A.; Bardhan, P.; Dowerah, D.; Mandal, M.; Deka, R.C. and Maji, T.K. Development of Rosin Derivative Crosslinked Vegetable Oil Based Keratin Fiber Reinforced Biodegradable Composites. *Waste Biomass Valorization*, 15(2): 787-803, 2023.

LIST OF BOOK CHAPTERS

- [1] Sarma, P. J.; Dowerah, D.; Biswakarma N. and Deka. R. C. Global Minimum Structures of (MnO)<sub>n</sub> clusters, *n* = 1-10 at DFT energy landscape. In *Air and Water Quality Assessment, Contamination and our Surroundings: Specific Analysis and Applications*, 20-42, 2019.
- [2] Deka, R.C.; Sarma, P.J.; Deka, A.; Biswakarma, N.; Dowerah, D. and Dey Baruah, S. Mechanistic Details of Catalytic Hydrogenation of CO<sub>2</sub> to Useful Chemicals Using SnO<sub>2</sub> Clusters. *Heterogeneous Nanocatalysis for Energy and Environmental Sustainability*, 2: 305-335, 2022.

LIST OF CONFERENCES AND SYMPOSIUMS ATTENDED

Year	Title of Conference	Institution	Mode of presentation (oral/poster)
2017	National Conference on “Nanomaterials Science, Technology and Applications” (NAMASTA-2017)	Dibrugarh University, Dibrugarh.	Poster (National)
2018	ORGANIX-218: An International Conference in Chemistry	Tezpur University, Tezpur.	Poster (International)
2019	Symposium on “Accelerating Biology 2019: Towards Thinking Machines”	C-DAC, Pune.	Poster (International)
2020	International Conference on “Emerging Trends in Chemical Sciences” (ETCS-2020)	Guwahati University, Guwahati.	Oral (International)
2022	National Conference on “Sustainability, Medicine and Clean Energy”	Tezpur University, Tezpur.	Poster (National)
2022	National Conference on “Recent Advances in Chemistry: Theoretical and Computational Aspects”	NEHU, Shillong & NIT Meghalaya	Poster (National)
2023	National Seminar on “Research at the Interface of Chemical Biological and Material Sciences”	Tezpur University, Tezpur.	Oral (National)

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