NSHM Knowledge Campus, Durgapur,

Research Publication

1. Riddhi Sainda, **Sourav Kanti Jana**, Prafulla K Jha. "Multiscale simulation of pesticides adsorption on passivated carbon nanotubes." *Diamond and Related Materials* (**IF:5.1, Q1**) 2026,163,113279.
   https://doi.org/10.1016/j.diamond.2025.113279
2. Thanasee Thanasarnsurapong, **Sourav Kanti Jana**, Panyalak Detrattanawichai, Waraporn Namunmong, Wisit Hirunpinyopas, Pawin Iamprasertkun, and Adisak Boonchun. "Accelerating Lattice Thermal Conductivity Calculations in MXenes: A Machine Learning Force Field Approach." *ACS Materials Au* **(IF:6.5, Q1)** 2025, 5, 5, 823-830.
   https://doi.org/10.1021/acsmaterialsau.5c00043
3. **Sourav Kanti Jana**, Thanasee Thanasarnsurapong and Adisak Boonchun. "Machine Learning-Guided Discovery of Multifunctional Nb_2CX_2 MXenes (X = S, Se, Te): Insights into Mechanical Properties and Thermal Conductivity." *Journal of Materials Chemistry C* (**IF: 5.7, Q1**) 2025, 13, 8631-8640.
   https://doi.org/10.1039/D4TC05430J
4. Ashvin Kanzariya, Narayan N Som, Shardul Vadalkar, **Sourav Kanti Jana**, LK Saini, Prafulla K Jha. "A First Principles exploration of pristine and p-block doped triangulene carbon dots for Hydrogen evolution reaction." *Molecular Catalysis* (**IF:3.9, Q2**) 2025, 572, 114766.
   https://doi.org/10.1016/j.mcat.2024.114766
5. **Sourav Kanti Jana**, Namrata A Tukadiya, Adisak Boonchun, Prafulla K Jha. "Metal–Metalloid Modified C_{36} Fullerene: A Dual Role in Drug Delivery and Sensing for Anticancer Chlormethine Explored through DFT and MD Simulations." *ACS Omega* (**IF:3.7, Q2**) 2024, 9, 50, 49786–49803.
   https://doi.org/10.1021/acsomega.4c08490
6. **Sourav Kanti jana**, Narayan N. Som, and Prafulla K. Jha "Size-dependent fullerenes for enhanced interaction of L-leucine: A combined DFT and MD Simulations approach." *Langmuir* (**IF:3.7, Q1**) 2024, 40, 27, 13844–13859.
   https://doi.org/10.1021/acs.langmuir.4c00806
7. Ashvin Kanzariya, Shardul Vadalkar, **Sourav Kanti Jana**, L. K. Saini1, and Prafulla K. Jha. "An Ab-initio Study for Adsorption of Hazardous CO_2, H_2S, HCN, and CNCl Molecules over Transition Metal-doped Graphene Quantum Dot". *Journal of Physics and Chemistry of Solids* (**IF:4.3, Q2**) 2024, 183,111799.
   https://doi.org/10.1016/j.jpcs.2023.111799
8. Tamalapakula, Vani, **Sourav Kanti Jana**, Narayan N. Som, Prafulla K. Jha, and Vijjulatha Manga. "Molecular Dynamic Simulation Studies on Cyclophilin-a Missing Cord in HIV-1 Capsid Assembly." (2023).
   https://doi.org/10.21203/rs.3.rs-2765729/v1.
9. Namrata A Tukadiya, **Sourav Kanti Jana**, Brahmananda Chakraborty, and Prafulla K. Jha. "C_{24} Fullerene and its Derivatives as a viable Glucose Sensor: DFT and TD-DFT studies." *Surfaces and Interfaces* (**IF:5.7, Q1**) 2023,41,103220.
   https://doi.org/10.1016/j.surfin.2023.103220.

10. **Sourav Kanti jana**, Narayan N. Som, and Prafulla K. Jha. “Theoretical appraisements on the interaction behavior of Amphetamine, Ketamine and Mercaptopurine drug molecules over C_{24} fullerene: A combined dispersion corrected DFT and MD simulation Study.” *Journal of Molecular Liquids* (**IF:5.3, Q1**) 2023,383,122084. https://doi.org/10.1016/j.molliq.2023.122084.

11. **Sourav Kanti Jana**, Darshil Chodvadiya, Narayan N. Som, and Prafulla K. Jha. “A quantum mechanical prediction of C_{24} fullerene as a DNA nucleobase biosensor.” *Diamond and Related Materials* (**IF:4.3, Q2**) 2022, 129, 109305. https://doi.org/10.1016/j.diamond.2022.109305.