List of publications

Related to Thesis:

1. Jana, Sourav Kanti, 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 129 (2022): 109305. https://doi.org/10.1016/j.diamond.2022.109305

2. Jana, Sourav Kanti, Narayan N. Som, and Prafulla K. Jha. "Theoretical appraisements on the interaction behaviour of amphetamine, ketamine and mercaptopurine drug molecules over C_{24} fullerene: A combined dispersion corrected DFT and MD simulation study." Journal of Molecular Liquids 383 (2023): 122084. https://doi.org/10.1016/j.molliq.2023.122084

3. Jana, Sourav Kanti, Narayan N. Som, and Prafulla K. Jha. "Size-dependent fullerenes for enhanced interaction of L-leucine: A combined DFT and MD Simulations approach." (Submitted to Journal)

Publication outside the scope of this thesis:

1. Tukadiya, Namrata A., 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 41 (2023): 103220. https://doi.org/10.1016/j.surfin.2023.103220

2. 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
3. Ashvin Kanzariya, Shardul Vadalkar, Sourav Kanti Jana, L. K. Saini1, and Prafulla K. Jha. "An Ab-initio Study for Adsorption of Hazardous CO2, H2S, HCN, and CNCl Molecules over Transition Metal-doped Graphene Quantum Dot". Journal of Physics and Chemistry of Solids (2023). (Accepted to "journal of physics and chemistry of solids")

Under preparation:

1. Jana Sourav Kanti, Narayan N. Som, and Prafulla K. Jha. "The binding affinity of pristine C_{36} fullerene towards anti-cancer drug chloromethane: Implications for drug delivery".

2. Jana Sourav Kanti, Nair T. Heera, Chakraborty Brahmananda and Prafulla K. Jha"Pristine and TM decorated Holey graphene as potential carriers for cisplatin drug delivery: A first Principles Study".