SAMBIT KUMAR DAS

CURRICULUM VITAE

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SKILLS:

- Computational Chemistry Tools: ORCA, Gaussian, OpenMolcas, Sharc, Molpro
- Programming Languages: Fortran, Python, Matlab, Shell Scripting
- Visualization Software Packages: Avogadro, Molden, PyMol, Chemdraw
- Operating Systems: Linux, Windows
- Others: Windows documentation and presentation
- Languages: English (Fluent), Hindi (Fluent), Odia (Native)

EDUCATION:

Doctor of Philosophy (Ph.D. Chemistry)
Stockholm University, Stockholm, Sweden
04/2021 – Present

Master of Science (M.Sc. Chemistry)
Indian Institute of Technology (IIT) Bhubaneswar, Odisha, India
05/2018 *CGPA: 9.41*

Bachelor of Science (B.Sc. Chemistry)
Fakir Mohan Autonomous College, Balasore, Odisha, India
04/2016 *Percentage: 82.33*

RESEARCH EXPERIENCES:

Simulation of excited state dynamics and transient X-ray spectra in solution (2021 – Present)

The aim of my Ph.D. work involves developing protocols for dynamical simulations of transient X-ray spectra of photoinduced processes in solution. In particular, modeling solvent polarization effect on the excited state dynamics and the X-ray absorption signal following charge-transfer excitations. Implementation of surface-hopping molecular dynamics simulations to treat non-adiabatic transitions in photo-induced processes. Quantum chemical treatment on the calculated trajectories will be done to determine the contributions from different electronic states. Such studies will provide better understanding of the excited state molecules undergoing bond dissociation and the valence-excited and core-excited states underlying the X-ray spectra.

High-throughput computation of molecular thermochemistry (2018 – 2020)

As a Research Fellow at the Tata Institute of Fundamental Research (TIFR), Hyderabad, I was working on *ab initio* quantum chemistry composite methods to determine thermochemical properties. Our focus was on the additivity approach adapted in the composite procedure, G4(MP2), and to propose strategies for reducing computational cost without compromising accuracy. The bigger picture behind this project was to develop a G4(MP2) variant that is applicable for high-throughput computation of thermochemical properties across small molecule chemical space.

Theoretical elucidation of chemical reactions using Intrinsic Reaction Coordinate (2017 – 2018)

As a part of my M.Sc. curriculum, I had carried out a year-long research work which was aimed to explain chemical reactions, from a quantum chemical point of view using the theory of IRC. The Diels-Alder addition was an integral part of the studied reactions and based on the results of the reaction coordinates, characterization of the reagents was done to get a better insight into the Diels-Alder reactions.

REFERENCES:

Prof. Michael Odelius
(Ph.D. supervisor)
"Professor, Stockholm University, SWEDEN"
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Prof. Raghunathan Ramakrishnan
(Project supervisor,
TIFR, Hyderabad)
"Reader, TIFR, Hyderabad, INDIA"
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Prof. Kousik Samanta
(M.Sc. project supervisor,
IIT, Bhubaneswar)
"Assistant Professor, IIT Bhubaneswar, INDIA"
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POSTER PRESENTATIONS:

"Rapid and Accurate Composite *ab initio* Models for High-throughput Computation of Molecular Thermochemistry across Chemical Space"

- Oct 2019, TACC-2019 (TIFR, Mumbai, India)
- Feb 2020, NSRAC-2020 (Pondicherry University, India)

PUBLICATIONS:

- S. K. Das, S. Chakraborty, R. Ramakrishnan, "Critical Benchmarking of Popular Composite Thermochemistry Models and Density Functional Approximations on a Probabilistically Pruned Benchmark Dataset of Formation Enthalpies" J. Chem. Phys. 154, 044113 (2021)

- S. K. Das, S. Senthil, S. Chakraborty, R. Ramakrishnan, "All Hands on Deck: Accelerating Ab Initio Thermochemistry via Wavefunction Approximations" (to be submitted) arXiv preprint: 10.26434/chemrxiv.14524890.v1