Koushik Naskar

Koushikphy | koushikphy111 | koushikphy.github.io
koushik.naskar9@gmail.com | Koushik Naskar

Education

2018 - 2024	**Ph.D.** in Theoretical & Computational Chemistry at *Indian Association for the Culitvation of Science, Kolkata*, (Thesis submitted) Expected date of degree: June, 2024	
2015 - 2017	**Master of Science (Physics)** at *Indian Institute of Technology, Guwahati*	(8.32/10.0)
2012 - 2015	**Bachelor of Science (Physics)** at *Presidency University, Kolkata*	(7.33/10.0)
2012	**Higher Secondary** at *Howrah Zilla School* (Affiliated to WBCHSE)	(84.40%)

Skills

Numerical Programming	Python (NumPy, SciPy, Pandas, Matplotlib etc.), C, C++, Fortran
High Performance Computing	OpenMP, MPI, CUDA (GPU), Job Scheduler (PBS, Slurm)
Machine Learning	Scikit-Learn, PyTorch, Neural Network, Deep learning, CNN, NLP, Time Series Analysis
Web Development	HTML, CSS, Javascript, React JS, NodeJS, Django, Flask, Dash-Plotly
Databases	SQLite, PostgreSQL, MongoDB
Software Development	Electron JS, Flutter
Miscellaneous	Git, Shell scripting, LaTeX, CI/CD

Projects & Experience

- Experience in developing and maintaining performance-critical large scientific codebases, with expertise in efficiently parallelizing them using OpenMP/MPI across hundreds of cores and nodes of computing cluster/supercomputer.
- Developed a highly parallelized software package for modelling Hamiltonian and determining their time-evolution using wave packet methodology for atom-diatom collision processes (Manuscript in preparation).
- *ADT*: A software package for constructing diabatic potential energy surfaces numerically and analytically employing beyond Born-Oppenheimer theory for any number of electronic states and nuclear degrees of freedom. (Published in *J. Chem. Theory Comput.*). *https://github.com/AdhikariLAB/ADT-Program*
- *PESMan*: A Python program package that greatly simplifies and enhances the construction of global potential energy surfaces. *https://github.com/Koushikphy/PESMan*
- *Interactive Data Editor*: A software built with Electron JS facilitating easy refinement and removal of irregularities from data graphically. *https://github.com/Koushikphy/Interactive_Data_Editor*
- Designed a Django web server for managing multiple Workstations/Clusters in a single place. *https://github.com/Koushikphy/System-Status-Checker*
- Developed an Android app that manages group shared expenses. *https://github.com/Koushikphy/Shared-Expense-Manager*

Research Publications

13. **K. Naskar**, S. Mukherjee, S. Ghosh and S. Adhikari, *J. Phys. Chem. A*, **128**, 1438 (2024)

12. M. K. Sah, S. Mukherjee, **K. Naskar**, S. Hazra and S. Adhikari, *Int. J. Quantum Chem.*, **123**, e27212 (2023)
11. S. Mukherjee[†], **K. Naskar**[†], S. Hazra, M. K. Sah and S. Adhikari *J. Phys. Conf. Ser.*, (accepted, 2023)
10. M. K. Sah, S. Mukherjee, S. Saha, **K. Naskar**, and S. Adhikari, *J. Chem. Phys.*, **159**, 244116 (2023)
9. **K. Naskar**, S. Ghosh, S. Adhikari, M. Baer and N. Sathyamurthy, *J. Chem. Phys.*, **159**, 034302, (2023)
8. **K. Naskar**, S. Ravi, S. Adhikari, M. Baer and N. Sathyamurthy, *J. Phys. Chem. A*, **127**, 3832, (2023)
7. J. Dutta, **K. Naskar**, S. Adhikari, J. Meyer and M. Somers, *J. Chem. Phys.*, **157**, 194112 (2022)
6. **K. Naskar**, S. Ghosh and S. Adhikari, *J. Phys. Chem. A*, **126**, 3311 (2022)
5. S. Mukherjee, S. Ravi, **K. Naskar**, S. Sardar and S. Adhikari *J. Chem. Phys.*, **154**, 094306 (2021)
4. J. Dutta, S. Mukherjee, **K. Naskar**, S. Ghosh, B. Mukherjee, S. Ravi and S. Adhikari, *Phys. Chem. Chem. Phys.*, **22**, 27496 (2020).
3. B. Mukherjee[†], **K. Naskar**[†], S. Mukherjee, S. Ravi, K. R. Shamsundar, D. Mukhopadhyay and S. Adhikari, *J. Chem. Phys.*, **153**, 174301/1-20 (2020)
2. **K. Naskar**[†], S. Mukherjee[†], B. Mukherjee, S. Ravi, S. Mukherjee, S. Sardar and S. Adhikari, *J. Chem. Theory Comput.*, **16**, 1666-1680 (2020).
1. **K. Naskar**, S. Mukherjee, S. Ghosh, T. Sahoo and S. Adhikari, *Int. Rev. Phys. Chem.*, **38**, 287 (2019).

([†]indicates equal contribution)

Awards and Scholarships

2020	CSIR-NET Senior Research Fellowship
2017	Graduate Aptitude Test in Engineering (GATE)
2015 & 2016	CSIR-NET Junior Research Fellowship
2015	Joint Admission to MSc (JAM)
2012	DST-INSPIRE Scholarship for Higher Education (SHE)
2010 & 2011	DST-INSPIRE SEATS Award & Internship