Koushik Naskar

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Google Scholar: Koushik Naskar
LinkedIn Koushik Naskar

Present Employment

2018 - Present	**Ph.D.** in Theoretical & Computational Chemistry Indian Association for the Culitvation of Science, Kolkata (Thesis submitted) Expected date of degree: May, 2024

Education

June 2017	**Master of Science** in Physics Indian Institute of Technology, Guwahati, CGPA: 8.32/10.0
July 2015	**Bachelor of Science** in Physics Presidency University, Kolkata, CGPA: 7.33/10.0
2012	**Higher Secondary** Howrah Zilla School, Affiliated to WBCHSE, Marks: 84.40%

Technical Skills

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

Development 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.

- *ADT*: A numerical and analytical software for constructing diabatic potential energy surfaces. (Published in *J. Chem. Theo. 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*)

- Designed a software that enables 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*)

Awards and Scholarships

February, 2017	Graduate Aptitude Test in Engineering (GATE)-2017
December, 2016, December, 2015	CSIR-NET Junior Research Fellowship
2012	DST-INSPIRE Scholarship for Higher Education (SHE)
2010 & 2011	INSPIRE Awards & Internship, DST-INSPIRE SEATS programme

Publications

1. Fully coupled 3D (J>0) Time Dependent Wave Packet calculation using Hypershperical Coordinates on diabatic surfaces of F+H_2,
Koushik Naskar, Soumya Mukherjee, Sandip Ghosh and Satrajit Adhikari,
Journal of Physical Chemistry A , DOI: https://doi.org/10.1021/acs.jpca.3c05590

2. Curl Condition: Existence of Sub-Hilbert Space for Molecular Species or Chemical Processes
Mantu Kumar Sah, Soumya Mukherjee, **Koushik Naskar**, Saikat Hazra and Satrajit Adhikari,
International Journal of Quantum Chemistry, **123**, e27212 (2023)

3. Beyond Born-Oppenheimer Treatment for Multi-State Photoelectron Spectra, Phase Transitions of Solids and Scattering Processes
Soumya Mukherjee[†], **Koushik Naskar**[†], Saikat Hazra, Mantu Kumar Sah and Satrajit Adhikari
([†]indicates equal contribution)
Journal of Physics: Conference Series, (accepted, 2023)

4. Photoelectron Spectra of Benzene: Can Path Dependent Diabatic Surfaces Provide Unique Observables?,
Mantu Kumar Sah, Soumya Mukherjee, Swagato Saha, **Koushik Naskar**, and Satrajit Adhikari,
Journal of Chemical Physics, **159**, 244116 (2023)

5. Coupled three-dimensional quantum mechanical wave packet study of proton transfer in H_2^+ + He collisions on accurate ab initio two-state diabatic potential energy surfaces **Koushik Naskar**, Sandip Ghosh, Satrajit Adhikari, Michael Baer and Narayanasami Sathyamurthy,
The Journal of Chemical Physics , **159**, 034302, (2023)

6. Beyond Born-Oppenheimer Constructed Diabatic Potential Energy Surfaces for HeH_2^+, **Koushik Naskar**, Satyam Ravi, Satrajit Adhikari, Michael Baer and Narayanasami Sathyamurthy,
Journal of Physical Chemistry A , **127**, 3832, (2023)

7. Effect of surface temperature on quantum dynamics of D_2 on Cu(111) using a chemically accurate potential energy surface
Joy Dutta, **Koushik Naskar**, Satrajit Adhikari, Joerg Meyer, and Mark Somers,
Journal of Chemical Physics, **157**, 194112 (2022)

8. Accurate Calculation of Rate Constant and Isotope Effect for F+H_2 Reaction by Coupled 3D Time-dependent Wave Packet Method on the Newly Constructed ab initio Ground Potential Energy Surface
Koushik Naskar, Sandip Ghosh and Satrajit Adhikari,
Journal of Physical Chemistry A, **126**, 3311 (2022)

9. A Beyond Born-Oppenheimer Treatment of $C_6H_6^+$ Radical Cation for Diabatic Surfaces: Photoelectron Spectra of its Neutral Analogue Using Time-Dependent Discrete Variable Representation
Soumya Mukherjee, Satyam Ravi, **Koushik Naskar**, Subhankar Sardar and Satrajit Adhikari
Journal of Chemical Physics, **154**, 094306 (2021)

10. The role of electron–nuclear coupling on multi-state photoelectron spectra, scattering processes and phase transitions,
Joy Dutta, Soumya Mukherjee, **Koushik Naskar**, Sandip Ghosh, Bijit Mukherjee, Satyam Ravi and Satrajit Adhikari,

Physical Chemistry Chemical Physics, **22**, 27496 (2020).

11. Beyond Born–Oppenheimer Constructed Diabatic Potential Energy Surfaces for F+H_2 Reaction,
Bijit Mukherjee[†], **Koushik Naskar**[†], Soumya Mukherjee, Satyam Ravi, K. R. Shamsundar, Debasis Mukhopadhyay and Satrajit Adhikari,
([†]indicates equal contribution)
Journal of Chemical Physics, **153**, 174301/1-20 (2020)

12. ADT: A Generalized Algorithm and Program for Beyond Born-Oppenheimer Equations of "N" Dimensional Sub-Hilbert Space
Koushik Naskar[†], Soumya Mukherjee[†], Bijit Mukherjee, Satyam Ravi, Saikat Mukherjee, Subhankar Sardar and Satrajit Adhikari,
([†]indicates equal contribution)
Journal of Chemical Theory and Computation, **16**, 1666-1680 (2020).

13. Beyond Born-Oppenheimer Theory for Spectroscopic and Scattering Processes
Bijit Mukherjee, **Koushik Naskar**, Soumya Mukherjee, Sandip Ghosh, Tapas Sahoo and Satrajit Adhikari,
International Reviews in Physical Chemistry, **38**, 287 (2019).

Seminar and Conference

1. **Structure and Dynamics: Spectroscopy and Scattering (SDSS-2023)** by IACS, Kolkata India
October 5-8, 2023
2. **25th International Conference on the Jahn-Teller Effect (JTE-2023) - Virtual** by York University, Canada
May 14-18, 2023
3. **Spectroscopy and Dynamics of Molecules and Clusters (SDMC-2022)** by IIIT Hyderabad, IIT Hyderabad and TIFR Hyderabad, India
November 10-13, 2022
4. **Theoretical Chemistry Meeting: Structure and Dynamics (TCMSD-2022)** by IACS, Kolkata, India
May 26-29, 2022
5. **Theoretical Chemistry Symposium (TCS 2021) - Virtual** by IISER Kolkata, IACS Kolkata, University of Kalyani and S.N Bose National Centre For Basic Sciences Kolkata, India
December 11-14, 2021
6. **Spectroscopy and Dynamics of Molecules and Clusters (SDMC-2020)** by BITS PIlani and IIT Jodhpur, India
February, 20-23, 2020
7. **Theoretical Chemistry Symposium (TCS 2019)** by BITS PIlani, India
February 13-16, 2019