Koushik Naskar

Koushikphy
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Present Employment

2018 – Present

Ph.D. in Theoretical & Computational Chemistry
Indian Association for the Culitvation of Science, Kolkata
Thesis title: Reaction Dynamics under Beyond Born-Oppenheimer Situations
(Thesis submitted) Expected date of degree: April, 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 Performance Computing:** OpenMP, MPI, CUDA (GPU), 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:** Git, Shell scripting, 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 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).

Development Experience (continued)

- *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 *Journal of Chemical Theory and Computation*).
  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

Awards and Scholarships

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

Research Publications

13. 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 , **128**, 1438 (2024)*

12. 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)*

11. 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)

10. 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)*

9. 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)*

8. 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)*

6. 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)*

5. 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)*

4. 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).*

3. 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)*

2. 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).*

1. 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).*

Seminars and Conferences

7. **Structure and Dynamics: Spectroscopy and Scattering (SDSS-2023)** by IACS, Kolkata India
October 5-8, 2023

6. **25th International Conference on the Jahn-Teller Effect (JTE-2023) - Virtual** by York University, Canada
   May 14-18, 2023

5. **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

3. **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

2. **Spectroscopy and Dynamics of Molecules and Clusters (SDMC-2020)** by BITS PIlani and IIT Jodhpur, India
   February, 20-23, 2020

1. **Theoretical Chemistry Symposium (TCS 2019)** by BITS PIlani, India
   February 13-16, 2019