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Koushik Naskar

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Objective

Machine Learning and Data Science enthusiast with a Ph.D. in Computational Chemistry, and nearly 10 years of experience in Python, C, Fortran and high-performance computing, seeking quantitative researcher or data scientist opportunities.

Education

2018 - 2024	**Ph.D.** in Computational Chemistry at *Indian Association for the Cultivation of Science, Kolkata*	
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, Predictive Analysis, Natural Language Processing, Time Series Analysis
Web Development	HTML, CSS, Javascript, React JS, NodeJS, Django, Flask, Dash-Plotly
Database	SQLite, PostgreSQL, MongoDB
Software Development	Electron JS, Flutter
Miscellaneous	Big Data (Spark), Git, Shell scripting, MS Excel, LaTeX, CI/CD

Experience

Doctoral Research Scholar, IACS, Kolkata, India

- Created "*ADT*", a **software package using Python and Fortran** to construct diabatic potential energy surfaces both numerically and analytically for any number of electronic states and nuclear degrees for freedom. Implemented OpenMP parallelization and HDF5 file I/O, achieving a ∼6x reduction in computation time. (Published in *J. Chem. Theory Comput.*). *https://github.com/AdhikariLAB/ADT-Program*
- Developed a **highly parallelized software** package using Fortran and C to perform quantum dynamics simulation of elementary chemical reactions in order to obtain reaction cross sections and rate constants. Discovered novel ways to parallelize using OpenMP and MPI schemes across hundreds of cores and nodes of computing cluster/supercomputer, enhancing efficiency by up to 4x. (Manuscript in preparation)
- Designed a parallel **Python automation tool** that substantially simplifies and improves the efficiency of constructing global potential energy, achieving a 10x performance boost. *https://github.com/Koushikphy/PESMan*
- Constructed multi-state diabatic Hamiltonian for several realistic molecular systems, such as H_3^+, HeH_2^+, $F+H_2$ etc. and carried out quantum wave packet simulations of the related chemical reactions, leading to several publications in various reputed international journals.

Data Science Projects

- Developed a comprehensive end-to-end **machine learning pipeline** for exploring, analyzing, and **predicting customer churn risk** at a bank. This involved extensive data processing, feature engineering and exploratory data analysis (EDA) to identify key predictors of churn. Utilized a Random Forest classifier with hyperparameter optimization, achieving an accuracy of 86% and a ROC-AUC score of 0.91.
- Conducted a **comprehensive study on obesity risk** factors, employing machine learning models such as Support Vector Machine (SVM), Random Forest, and K-Nearest Neighbors (KNN) for multi-class classification. Achieved a top accuracy score of 90% by performing thorough feature selection and engineering. Implemented cross-validation and ensemble methods to improve model generalization and robustness.

- Developed a Convolutional Neural Network (CNN) model leveraging transfer learning to **classify paddy diseases** from images. Employed advanced techniques such as data augmentation and fine-tuning of pre-trained model (ResNet) to improve the model's ability to generalize across diverse datasets, achieving a high accuracy rate of 96%
- Applied the ARIMA model for **time series forecasting**, accurately predicting trends and patterns in financial sales datasets. Conducted rigorous time series analysis, including stationarity testing, seasonality decomposition, and autocorrelation function (ACF) analysis, to select appropriate model parameters.
- Performed extensive **regression analysis**, following data visualization and feature engineering, to accurately predict the age of abalones, achieving a RMSLE score of 0.17.

Master's Student, IIT Guwahati

- Developed efficient codes in Python and Fortran for **simulating and visualizing** the formation and dissociation of Hydrogen bonds in water in the presence of ions, **using Molecular Dynamics**. Employed parallel computing to enhance performance, significantly reducing simulation time.

Other Projects

- *Interactive Data Editor*: Designed an innovative graphical approach for **simplifying data cleaning**. Built with Node JS and Electron JS for cross-platform compatibility. Deployed **CI/CD pipelines** using GitHub Actions to automate the building and deployment of software binaries across various operating systems and platforms. *https://github.com/Koushikphy/Interactive_Data_Editor*
- *TeleJobReminder*: Created a **Telegram bot** using **Python Flask, PostgreSQL** and Telegram API to monitor and manage computer jobs. The bot tracks job statuses and sends notifications upon completion or failure, providing real-time updates to users. Deployed on the cloud.
  https://github.com/Koushikphy/TeleJobReminder
- Built a **Django web server** with a comprehensive dashboard for the efficient management of multiple workstations and clusters.
  https://github.com/Koushikphy/System-Status-Checker
- *kbib*: Crafted a **Python tool** that generates academic references from DOIs or PDFs in various formats by utilizing the CrossRef R**EST API**, enhancing efficiency for researchers and academicians. Deployed it on PyPI for easy access. *https://github.com/Koushikphy/kbib*

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

Research Publications

14. On the quantum dynamical treatment of surface vibrational modes for reactive scattering of H_2 from Cu(111) at 925 K,
    M. K. Sah, K. Naskar, S. Adhikari, B. Smits, J. Meyer and M. Somers *J. Chem. Phys.*, **161**, 014306 (2024)
13. Coupled 3D (J≥0) Time Dependent Wave Packet Calculation for F+H_2 Reaction on Accurate *Ab Initio* Multi-State Diabatic Potential Energy Surfaces,
    K. Naskar, S. Mukherjee, S. Ghosh and S. Adhikari, *J. Phys. Chem. A*, **128**, 1438 (2024)
12. Beyond Born-Oppenheimer Treatment for Multi-State Photoelectron Spectra, Phase Transitions of Solids and Scattering Processes,

S. Mukherjee†, K. Naskar†, S. Hazra, M. K. Sah and S. Adhikari, *J. Phys. Conf. Ser.*, **2769**, 012012, (2024)

11. Curl Condition: Existence of Sub-Hilbert Space for Molecular Species or Chemical Processes,
M. K. Sah, S. Mukherjee, K. Naskar, S. Hazra and S. Adhikari, *Int. J. Quantum Chem.*, **123**, e27212 (2023)

10. Photoelectron Spectra of Benzene: Can Path Dependent Diabatic Surfaces Provide Unique Observables?,
M. K. Sah, S. Mukherjee, S. Saha, K. Naskar, and S. Adhikari, *J. Chem. Phys.*, **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,
K. Naskar, S. Ghosh, S. Adhikari, M. Baer and N. Sathyamurthy, *J. Chem. Phys.*, **159**, 034302, (2023)

8. Beyond Born-Oppenheimer Constructed Diabatic Potential Energy Surfaces for HeH_2^+,
K. Naskar, S. Ravi, S. Adhikari, M. Baer and N. Sathyamurthy, *J. Phys. Chem. 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,
J. Dutta, K. Naskar, S. Adhikari, J. Meyer and M. Somers, *J. Chem. Phys.*, **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,
K. Naskar, S. Ghosh and S. Adhikari, *J. Phys. Chem. 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,
S. Mukherjee, S. Ravi, K. Naskar, S. Sardar and S. Adhikari, *J. Chem. Phys.*, **154**, 094306 (2021)

4. The Role of Electron-Nuclear Coupling on Multi-State Photoelectron Spectra, Scattering Processes and Phase Transitions,
J. Dutta, S. Mukherjee, K. Naskar, S. Ghosh, B. Mukherjee, S. Ravi and S. Adhikari,*Phys. Chem. Chem. Phys.*, **22**, 27496 (2020).

3. Beyond Born-Oppenheimer Constructed Diabatic Potential Energy Surfaces for F + H_2 Reaction,
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. ADT: A Generalized Algorithm and Program for Beyond Born-Oppenheimer Equations of "N" Dimensional Sub-Hilbert Space,
K. Naskar†, S. Mukherjee†, B. Mukherjee, S. Ravi, S. Mukherjee, S. Sardar and S. Adhikari, *J. Chem. Theory Comput.*, **16**, 1666-1680 (2020).

1. Beyond Born-Oppenheimer Theory for Spectroscopic and Scattering Processes,
B. Mukherjee, K. Naskar, S. Mukherjee, S. Ghosh, T. Sahoo and S. Adhikari, *Int. Rev. Phys. Chem.*, **38**, 287 (2019).

(†indicates equal contribution)

Certificates

- PyTorch for Deep Learning with Python Bootcamp
- Python for Data Science and Machine Learning Bootcamp
- Django 3 - Full Stack Websites with Python Web Development