Ajay Khanna

Ph.D., Computational Chemist
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Summary

An aspiring postdoctoral researcher with a Ph.D. in Computational Chemistry, specializing in the intersection of computational physics and chemistry, focusing on optical spectroscopy, resonance energy transfer, excited state properties, and dynamics of molecules in a condensed environment. Expertise in high-throughput computational techniques, spanning ground and excited state ab initio molecular dynamics, with a strong foundation in high-performance and GPU computing. Adept using Cheminformatics tools for advanced high-throughput virtual screening and ML applications. Bringing industrial experience in developing rank-ordering computational pipelines for accelerating rank-ordering potential molecules. Excellent writing, communication, and collaboration, evident from successful resource allocation grants, oral presentations, and experimental collaborations.

Education

- **Ph.D**. Computational Chemistry, University of California, Merced, July 2024
- **M.Sc**. Chemistry and Chemical Biology, UC Merced, California, USA, May 2022
- **M.Sc**. Chemistry, National Institute of Technology (NIT), Rourkela, India, May 2017
- **B.Sc**. Chemistry (Hons.), University of Delhi, New Delhi, India, July 2015

Professional certification

- Introduction to Cheminformatics and Medicinal Chemistry, Udemy
- Data Science with Python, Simplilearn
- Fundamental of Accelerated Computing with CUDA Python, NVIDIA

Work Experience

Ph.D. Computational Chemistry, Advisor: Dr. **Christine Isborn**, Place: UC Merced, *CA,* *Aug.2018 – July.2024*

- **Developed** computational absorption and fluorescence spectroscopy methods to accurately reproduce experimental spectra of molecules using hybrid quantum mechanics and molecular dynamics in condensed environments, leading to a deeper understanding of the role of configurational space, choice of theoretical methods, and explicit environmental effects on molecules' spectroscopic properties.
- **Developed** methods combining ensemble sampling with excitonic coupling methods to compute the rate of energy transfer processes between ligands used in bioimaging. Provided a path for understanding the role of environmental impact in controlling the energy transfer processes.
- **Developed** open-source Python code to compute molecules' vibrational frequencies and fluorescence spectra in explicit solvents, interfaced it with TeraChem and Gaussian, and integrated it into **MolSpeckPy**.
- **Collaborated** with experimental chemists and physicists on a new field of chemistry, Polariton, a $7.5 million DOD-funded project. Using absorption spectroscopy, ab initio molecular dynamics, and charge transfer analysis linked experimental results to quantum mechanical properties of the J & H aggregates.
- **Managed** local HPC clusters, including installing CUDA libraries and CUDA-based QM software. Automated large-scale molecular dynamics jobs using Slurm, bash, and Python scripts. Efficiently scaled high-throughput jobs at least twofold.

CADD Intern, Advisor: Dr. **Monika Williams**, Place: Frontier Medicines, South San Francisco*, CA, May 2023 – Aug.2023*

- **Actively** participated in live **KRAS-G12C** modeling meetings with multidisciplinary teams of MedChem and the synthetic Chemist and provided insight on Structure-based drug design, such as pKa and lipophilicity.
- **Utilized** MOE for ligand docking in protein structures and **developed** computational pipelines for SMILES processing and protein-ligand binding free energy calculations using hybrid QM/MM techniques**.**
- **Collaborated** in interdisciplinary teams of Medicinal Chemists, Discovery biologists, Pharmacologists, and Crystallographers, contributing to structural-based drug design discussions and enhancements.

Teaching Assistant, Place: UC Merced *Aug.2018 – Dec.2022*

- Taught introductory chemistry courses (> 95% 1st gen students) and prepared worksheet materials for four years.

Research Intern, Advisor**: Dr. Biman Bagchi,** Place**:** Indian Institute of Science, Bangalore *Jan.2018 – July.2018*

- Modeled absorption and fluorescence spectra of Alexa Fluor dyes in implicit solvents. Performed functional benchmarks with DFT and TDDFT levels of theory.

Research Intern, Advisor: **Dr. Ayan Datta,** Place**:** Indian Association for the Cultivation Science, Kolkata *Aug.2017 – Nov.2017*

- **Developed** a computational molecular dynamics procedure to generate 3D DNA origami nanostructures using CadNano and oxDNA**,** later used to generate unique metal clusters.

Research Assistant, Advisor**: Dr. Santanab Giri,** Place**:** NIT Rourkela *July 2016 – July.2017*

- **Conducted** quantum mechanical investigation of Zintl phases, showed 18-electron rule's ability to predict and design better Zintl ions and Zintl phases with better magnetic properties.

Intern, Advisor**: Dr. Debashree Ghosh,** Place**:** National Chemical Laboratories, Pune *May 2016 – July.2016*

- Worked on understanding the application of effective fragment potential (EFP) methods for computing the electronic properties of GFP protein with various fragments.

Skills

- **Quantum Mechanics (QM)** Techniques: Hybrid QM/MM, HF, DFT/TDDFT/DFTB/LC-DFTB, Spectroscopy, Solvent Chemistry: Implicit and Explicit, Minimization, FRET, Charge Transfer Analysis, and Force Field Parameterization
- **Molecular Dynamics (MD)** Techniques: Ab initio MD, Ground and excited State, classical, and Enhanced sampling.
- **Drug Discovery** Techniques**:** Free energy: QM/MM, TI, MM-P(G)BSA, Docking, Protein-Ligand interaction, Similarity search, and Structure-based drug design.
- **Machine Learning**: Linear regression, Decision Trees, Random Forest, k-mean clustering, and GNNs
- **Programming**: Python, C++, Bash, and CUDA@numba
- **Data Analysis**: NumPy, Pandas, Scikit-learn, SciPy, Plotly, Matplotlib, MDTraj, Vortex, and Excel
- **Cheminformatics:** Rdkit, CppTraj, OEChem and Open Babel
- **Simulation Packages:** Amber, OpenMM, Gromacs, Gaussian, TeraChem, MOE, Psi4, VMD, and Qubekit

Academic Publications

- **Ajay Khanna,** Christine M. Isborn, Resonance Energy Transfer Processes in Explicit Solvent Environment: Going Beyond Traditional FRET (On Going, Fall **2024)**
- **Ajay Khanna,** Sapana V. Shedge, Tim J. Zuehlsdorff, Christine M. Isborn; Calculating absorption and fluorescence spectra for chromophores in solution with ensemble Franck–Condon methods. **J. Chem. Phys**.; 161 (4): 044121, DOI:10.1063/5.0217080
- Christopher A. Myers, Shao-Yu Lu, Sapana Shedge, Arthur Pyuskulyan, Katherine Donahoe, **Ajay Khanna**, Liang Shi, and Christine M. Isborn, Axial H-bonding Solvent Controls Inhomogeneous Spectral Broadening, Peripheral H-bonding Solvent Controls Vibronic Broadening: Cresyl Violet in Methanol, J. Phys. Chem. B 2024, 128, 23, 5685–5699, DOI:10.1021/acs.jpcb.4c01401
- Chiao-Yu Cheng, Nina Krainova, Alyssa Brigeman, **Ajay Khanna**, Sapana Shedge, Christine Isborn, Joel Yuen-Zhou, and Noel C. Giebink, Molecular Polariton Electroabsorption, ***Nat Commun*** 13, 7937, 2022, DOI:10.1038/s41467-022-35589-4
- Sapana V. Shedge, Tim J. Zuehlsdorff, **Ajay Khanna**, Stacey Conley, and Christine M. Isborn, Explicit Environmental and Vibronic Effects in Simulations of Linear and Nonlinear Optical Spectroscopy, ***J. Chem. Phys***. 154, 084116, 2021, DOI: 10.1063/5.0038196
- Rakesh Parida, G. Naresh Reddy, **Ajay Khanna**, Gourisankar Roymahapatra and Santanab Giri, Ligand Driven Electron Counting Rule Selection: A Case Study for Ge_5R Complex, **Int. J. Hit. Tranc: Eccn**. Vol.4: Issue 1A, 2018, ISSN: 0973-6875

Grants

XSEDE/ACCESS **National HPC Grant**: Computational resources, **8000 GPU-hours**, **3000 CPU-hours**, worth **$5263** for efficiently scaling and running high-throughput computational jobs on San Diego Super Clusters.

National and International Conference Proceedings

- **Ajay Khanna**, Combining Ensemble and Franck-Condon Methods to Compute Absorption and Fluorescence Spectra of Molecules in Explicit Environment, West Coast Theoretical Chemistry (WCTC) UC Merced, Spring 2024 *(Poster)*
- Ajay Khanna, Modeling the Emission Spectrum of Molecules in the Explicit Environment, *ACS, Spring 2022 (Talk)*
- Ajay Khanna, Improved Methods for Modeling F(RET) in Complex Environment, *Department of Chemistry and Chemical Biology, UC Merced, Spring 2021 (Talk)*
- Ajay Khanna, Modeling Explicit Environment Effects on Emission Spectra and Excitation Energy Transfer, *ACS 2021 (Poster & Talk, Online)*

Awards

- Outstanding Graduate Student Support Award, UC Merced, 2023
- GROW TA Training and Support Fellowship, 2022
- Graduate Fellowship Incentive Program Award, 2022
- Graduate Excel Peer Mentor Award, 2022
- Chemistry Graduate Student Travel Award, 2022
- Summer Research Fellowship, UC Merced, 2019 and 2020

Professional Development Activities

Organizational Skills

- Machine learning Tutorial - Detecting functional groups in IR spectra Using Decision Trees and Random Forest, JCTC group, UC Merced, *Fall 2023*
- Python Bootcamp, Electronic Structure Calculations in Pure Python - Understanding Fundamentals with Python, JCTC group, UC Merced, *Fall 2021*
- Head organizer, Joint Computation and Theory Club (JCTC), *Aug.2021 – May.2022*
- Joint Secretary, Department of Chemistry, Ramjas College, University of Delhi, *Aug.2011 – Aug.2012*

Mentorship

- GradEXCEL Program, UC Merced: Abigail Gyamfi, Arthur Pyuskulyan, Aneelman Brar, Samaneh Farimand, Remi Leano, Pin Lyu, Indar and Ethan, *Aug.2019 - May.2022*

Teaching Pedagogy

- Certificate: Level 2: Principles of Pedagogy: Effective strategies for teaching, *Fall 2021*
- Certificate: Level 3: Advanced Pedagogy: Preparing future instructors' teaching career, *Spring 2022*

Communication

- Toastmasters, x5 best speech accolade (Local Club)
- Stanford, Writing in Sciences course by Dr. Kristin Sainani, peer-reviewed, scored 96.07%, *Jan.2021 – Mar.2021*