Anshuman Kumar, Ph.D.

Computational Materials Scientist with 6+ years of experience using theory and computation for complex problems

(951) 758-9673 | Riverside, CA | dranshuman.ai@gmail.com | anshuman | anshuman5 | Scholar | Portfolio

EDUCATION

University of California, Riverside **Sep. 2017 – Mar. 2023**
Ph.D. in Computational Materials Science *Riverside, CA*
Dissertation: Harnessing Large-Scale Quantum Calculations for Predicting Material and Chemical Properties

University of California, Riverside **Sep. 2015 – Aug. 2017**
Masters in Electrical Engineering, GPA – 3.80 *Riverside, CA*

TECHNICAL SKILLS

Languages: Python (Pandas, Matplotlib, NumPy, SciPy, Jupyter), Bash, SQL, C/C++, Java, CUDA
Technologies/Frameworks: Linux/Unix, GitHub, Git, Docker, Plotly, Dash, Azure
Machine Learning: TensorFlow, PyTorch, Scikit-learn, Neural Networks, Deep Learning, Transfer Learning
Simulation Tools: Vasp, Gaussian, Fhi-aims, Siesta, DFTB+, Materials Studio, Crystal17, CP2K, NWChem, Pymatgen, Casm, Plumed, GROMACS

EXPERIENCE

Postdoctoral Scholar June 2024 – Present
University of California *Davis, CA*
- Development, implementation and integration of multiscale molecular modeling methods with machine learning approaches to investigate the mechanisms of catalyst deactivation.

Subject Matter Expert June 2024 – Aug 2024
OpenAI *San Francisco, CA*
- Subject Matter Expert in Computational Sciences (Physics, Chemistry, Materials), Fluid Dynamics, Robotics, and programming. Prompt engineering, evaluation, and improving large language models (LLMs) through human-data.

Postdoctoral Scholar July 2023 – May 2024
University of California *Riverside, CA*
- Development of Regression (LASSO and Ridge) and generative AI (GAN, Diffusion) models to predict the band gap of 1-D and 2-D polymers based on their composition and crystal structure.
- Enabling Clustering Algorithm (PCA, t-SNE, DBSCAN) for the screening of multi-principal elements and high-entropy alloys, which are novel materials with high performance and stability.
- Optimization and development of machine learning deep potential in Density Functional Theory (DFT) and molecular dynamics calculations.

Software Engineer June 2011– Aug. 2015
Accenture *Bangalore, India*
- Led a 4-person team for the development and deployment of a web application for Cisco (San Jose, CA) using Java, contributing to the successful delivery of a critical project.
- Derived insights into user behavior using Data Analysis with Python and SQL.
- Designed and implemented phishing security vulnerabilities on web browsers using Javascript.
- Translated business requirements into technical specifications.

Research Assistant Sep. 2019 – Mar. 2023
University of California *Riverside, CA*
- Developed a customized docker image incorporating GPU-enabled density functional tight binding, with Plumed and Magma, on the Azure cloud platform. Utilized this image to perform molecular dynamics simulations for accurate evaluation of free energy surfaces of drug molecules.
- Applied electronic structure calculations in conjunction with Boltzmann transport calculations to determine the conductivity, mobility, and band structure of DNA.
- Developed and implemented a cutting-edge deep learning model to accurately predict time-dependent control fields, enabling precise manipulation of electronic transitions in quantum systems.
- Implemented quantum control algorithm for inverse problems in quantum mechanics and accelerated control of multi-qubit system with hamiltonian transformations.

- Conducted extensive evaluations of oligopeptides' UV circular dichroism and absorption spectra by employing the time-dependent density functional theory approach using Gaussian.
- Analyzed the linear polarizability and second hyperpolarizability using CCSD(T) and range-separated functionals on streptocyanines using Gaussian.
- Experience using high-performance computing clusters (Example: San Diego access supercomputers, Texas stampede clusters, and John Hopkins's rockfish).
- Published 11 peer-reviewed journal articles, 1 book chapter, and 2 conference proceedings during my Ph.D.

AWARDS

Dissertation Year Program Fellowship **June 2021 and June 2022**
University of California *Riverside, CA*

Department Fellowship, Materials Science and Engineering Program **Sep. 2017**
University of California *Riverside, CA*

TALKS

Argonne National Laboratory **Online (Zoom)**
Harnessing Large-Scale Quantum Calculations for Predicting Material and Chemical Properties *Nov 2023*

Dept. of Energy (DOE) Review Meeting of Crosscutting Technologies **Online (Zoom)**
Large-Scale, GPU-Enhanced DFTB Approaches for Probing Multi-Component Alloys *June 2021, Sept 2021*

DOE Review Meeting of Crosscutting Technologies **Pittsburgh, PA**
Large-Scale, GPU-Enhanced DFTB Approaches for Probing Multi-Component Alloys *Apr 2019*

REFERENCES

Prof. Bryan M. Wong, brwong@ucr.edu **951-827-2153**
University of California, Riverside

Prof. Reinhard Schweitzer-Stenner, rschweitzer-stenner@drexel.edu **215-895-2268**
Drexel University, Philadelphia

Prof. Chao Lian, chaolian@iphy.ac.cn
Institute of Physics, Chinese Academy of Sciences

SELECTED PUBLICATIONS

[1] **Anshuman Kumar**, Pablo R Arantes, Aakash Saha, Giulia Palermo, and Bryan M Wong. GPU-Enhanced DFTB Metadynamics for Efficiently Predicting Free Energies of Biochemical Systems. Molecules, 28(3):1277, 2023. URL https://doi.org/10.3390/molecules28031277.

[2] **Anshuman Kumar**, Zulfikhar A. Ali, and Bryan M. Wong. Efficient Predictions of Formation Energies and Convex Hulls from Density Functional Tight Binding Calculations. J. Mater. Sci. Technol., 141:236–244, 2023. ISSN 1005-0302. URL https://doi.org/10.1016/j.jmst.2022.10.002.

[3] **Anshuman Kumar**, Xian Wang, Christian R. Shelton, and Bryan M. Wong. Harnessing Deep Neural Networks to Solve Inverse Problems in Quantum Dynamics: Machine-Learned Predictions of Time-Dependent Optimal Control Fields. Phys. Chem. Chem. Phys., 22:22889–22899, 2020. doi: 10.1039/D0CP03694C. URL http://dx.doi.org/10.1039/D0CP03694C.

[4] Xian Wang, Mahmut Sait Okyay, **Anshuman Kumar**, and Bryan M Wong. Accelerating Quantum Optimal Control of Multi-Qubit Systems with Symmetry-Based Hamiltonian Transformations. AVS Quantum Science, 5 (4), 2023. URL https://doi.org/10.1116/5.0162455.

[5] Akber Raza, Chengkuan Hong, Xian Wang, **Anshuman Kumar**, Christian R Shelton, and Bryan M Wong. NIC-CAGE: An Open-Source Software Package for Predicting Optimal Control Fields in Photo-Excited Chemical Systems. Computer Physics Communications, 258:107541, 2021. URL https://doi.org/10.1016/j.cpc.2020.107541.