Anshuman Kumar, Ph.D.

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

(951) 758-9673 | Riverside, CA | anshuman.kumar@email.ucr.edu | 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 — *Riverside, CA*

Manipal Institute of Technology, Manipal — **Sep. 2007 – Aug. 2011**
Bachelors in Electronics and Communication Engineering — *Karnataka, India*

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, Mace, DeepMD-Kit

EXPERIENCE

AI Researcher — June 2024 – Present
OpenAI — *San Francisco, CA*
- Prompt engineering, evaluation, and improving large language models (LLMs).

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.

Postdoctoral Research Associate — July 2023 – Present
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.

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.
- Analyzed the linear polarizability and second hyperpolarizability using CCSD(T) and range-separated functionals on streptocyanines using Gaussian.
- Applied electronic structure calculations in conjunction with Boltzmann transport calculations to determine the conductivity, mobility, and band structure of DNA.
- Conducted extensive evaluations of oligopeptides' UV circular dichroism and absorption spectra by employing the time-dependent density functional theory approach using Gaussian.
- 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.
- Published 11 peer-reviewed journal articles, 1 book chapter, and 2 conference proceedings during my Ph.D.

Graduate Researcher — Sep. 2017 – Sep. 2019
University of California — *Riverside, CA*

- Utilized the Non-equilibrium Green's Function approach to model the *ab-initio* transport properties of a doped carbon nanotube network in a two-dimensional configuration.
- Experience using high-performance computing clusters (Example: San Diego access supercomputers, Texas stampede clusters, and John Hopkins's rockfish).

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.

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

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**, Siobhan E. Toal, David DiGuiseppi, Reinhard Schweitzer-Stenner, and Bryan M. Wong. Water-Mediated Electronic Structure of Oligopeptides Probed by Their UV Circular Dichroism, Absorption Spectra, and Time-Dependent DFT Calculations. The Journal of Physical Chemistry B, 124(13):2579–2590, 2020. URL `https://doi.org/10.1021/acs.jpcb.0c00657`.

[4] **Anshuman Kumar**, Reinhard Schweitzer-Stenner, and Bryan M. Wong. A New Interpretation of the Structure and Solvent Dependence of the Far UV Circular Dichroism Spectrum of Short Oligopeptides. Chem. Commun., 55:5701–5704, 2019. URL `http://dx.doi.org/10.1039/C9CC01513B`.

[5] **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.

[6] Hyuna Kwon, **Anshuman Kumar**, Mauro Del Ben, and Bryan M Wong. Electron/Hole Mobilities of Periodic DNA and Nucleobase Structures from Large-Scale DFT Calculations. The Journal of Physical Chemistry B, 2023. URL http://dx.doi.org/10.1021/acs.jpcb.2c09141.

[7] Lihua Xu, **Anshuman Kumar**, and Bryan M. Wong. Linear Polarizabilities and Second Hyperpolarizabilities of Streptocyanines: Results from Broken-Symmetry DFT and New CCSD(T) Benchmarks. Journal of Computational Chemistry, 39(28):2350–2359, 2018. URL http://dx.doi.org/10.1002/jcc.25519.

[8] Sarah I Allec, **Anshuman Kumar**, and Bryan M Wong. Linear-Response and Real-Time, Time-Dependent Density Functional Theory for Predicting Optoelectronic Properties of Dye-Sensitized Solar Cells. In Dye-Sensitized Solar Cells, pages 171–201. Elsevier, 2019. URL https://doi.org/10.1016/B978-0-12-814541-8.00005-7.

[9] Mingguang Chen, Wangxiang Li, **Anshuman Kumar**, Guanghui Li, Mikhail E. Itkis, Bryan M. Wong, and Elena Bekyarova. Covalent Atomic Bridges Enable Unidirectional Enhancement of Electronic Transport in Aligned Carbon Nanotubes. ACS Applied Materials & Interfaces, 11(21):19315–19323, 2019. URL https://doi.org/10.1021/acsami.9b01400.

[10] 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.

[11] 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.

[12] Yongho Joo, Lifeng Huang, Naresh Eedugurala, Alexander E London, **Anshuman Kumar**, Bryan M Wong, Bryan W Boudouris, and Jason D Azoulay. Thermoelectric Performance of an Open-Shell Donor–Acceptor Conjugated Polymer Doped with a Radical-Containing Small Molecule. Macromolecules, 51(10):3886–3894, 2018. URL https://doi.org/10.1021/acs.macromol.8b00582.