NAMAN KATYAL Ph.D.

Computational Expert in Atomistic and Machine Learning Materials Modeling
Lawrence Berkeley National Laboratory

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A results-driven Ph.D. researcher with expertise at the intersection of applied machine learning, cheminformatics, and computational chemistry. Proven track record architecting and building end-to-end ML solutions, including an LLM-powered toolkit for scientific literature recommendation. Proficient in PyTorch and TensorFlow , with extensive experience applying foundational and generative models to solve large-scale research problems. Passionate about creating open-source toolkits and leading collaborative, interdisciplinary research.

Technical Proficiencies

- **AI/ML Frameworks:** PyTorch, TensorFlow, Scikit-learn, Foundational Models, Generative Models.
- **Development & HPC:** C++, Git, SLURM, High-Performance Computing.
- **Simulation & Workflow Software:** Python, VASP, LAMMPS, Pymatgen, ASE, MatterSim, CHGNET, MACE, Orca, DFTB, VASPKIT, OQMD, Alamode, FEFF.
- **Force Field Development:** ML-driven force fields (PyAMFF, ACE), fine-tuning (CHGNET).
- **Computational Methods:** High-Throughput DFT, Force Field Development, Excited state ab-initio calculations (BSE, RPA), Molecular Dynamics, Monte Carlo Methods.

Relevant Experience

Lawrence Berkeley National Laboratory — ***Berkeley, CA***
Postdoctoral Researcher — 2023-Present

- **Lead Developer: High-throughput Materials Diffusion Toolkit (AI-ML)**
  - Architected and built a standalone modular toolkit for defect simulation and self-diffusion calculator in inorganic materials using MatterSim and MatterGen.
  - Automated defect structure generation, nudged-elastic band and diffusion pre-factor calculator. *Published on **Github**.*
- **Lead Developer: LLM-Powered Research Recommender Toolkit (AI-ML-LLM):**
  - Architected and built a standalone toolkit using Large Language Model to generate customized summaries and recommendations for scientific literature, demonstrating experience with NLP and data representation.
  - Published the tool on **GitHub**, showcasing end-to-end software engineering and open-source contribution.
- **Lead Developer: High-throughput Defect Structure Setup (AI-ML)**
  - Architected and built a standalone toolkit for defect structure generation and VASP input file generation in a given material.
  - VASP input files with spin polarized, correct magnetic ordering and on-site correction calculation can be setup for all defect orderings which is not possible with any given simulation package. *Published on **Github**.*
- **Engineered Scalable ML Workflows (AI-ML):**
  - Engineered and deployed scalable, data-driven ML workflows to predict system evolution and identify optimal pathways from vast, high-dimensional datasets. This automated workflow accelerated the discovery process significantly**.** Published in ACS Materials Letters.
- **Built Predictive Models for Accelerated Discovery (AI-ML):**
  - Created predictive models for phase transformation and ionic diffusion, significantly accelerating the discovery of efficient lithium extraction methods for climate-relevant energy storage. *Manuscripts under review as well as preparation.*

The University of Texas at Austin — ***Austin, TX***

- **Contributor: Accelerated DFT Code (*HPC/Scientific Computing*):**
  - Contributed to the highly scalable, open-source Socorro Density Functional Theory (DFT) code for extended systems, a key tool in computational materials science.
  - Developed and implemented a module for dynamical matrix calculations to complement Nudged Elastic Band (NEB) transition state searches, enabling the accurate determination of entropic pre-factors for self-diffusion processes.
- **Development of machine learning package PyAMFF (*AI-ML*)**
  - Created and optimized a novel ML force field package (**PyAMFF**) in PyTorch, achieving a 2x training speed-up on GPUs. *Published in Compute Physics Communications*
  - A Lithium machine-learned potential using PyAMFF with lowest reported 4meV/atom and 32 meV/atom/Å training and testing errors to study defect formation and transport in battery anodes over experimental timescales which involved massive data collection using geometry optimizations, ab-initio molecular dynamics, adaptive Kinetic Monte Carlo, and transition state searches.
- **Computational and experimental investigation of chlorine and bromine intercalated cathode host for dual-ion batteries (*AI-ML*)**
  - Density functional theory calculations found 0.08V vs Li/Li^+ difference in chlorine gas evolution and intercalation in graphite compared to 0.3V vs Li/Li^+ difference in bromine explaining enhanced performance of bromine-intercalated graphite cathodes in dual ion batteries.
  - Using materials databases and universal MACE ML potential, 4V and 350-500 Wh/kg energy density cathode hosts were screened for cheaper and high-energy density chloride-ion based dual-ion batteries. *Manuscript under preparation.*
- **Applied Advanced Computational Models to Predict Optical Properties**
  - Compared to bulk niobium oxides, computational Raman spectra discovered response at 648 cm^{-1} in 2-d synthesized niobium oxide structures instead of 900 cm^{-1} resulting in dimensionality dependent electrochromism.
  - Utilized DFT and beyond-DFT methods (RPA) to model how lithium intercalation creates tunable light absorption from near-IR to visible wavelengths (900nm to 500nm), a core requirement for near-eye display technology. *Published in: J. Am. Chem. Soc.* and *ACS Nano.*
- **Computational investigation of as-synthesized bimetallic clusters for ORR in zinc-air battery**
  - Using experimental XRD and EXAFS, Fe-Ni bimetallic clusters were modeled using density functional theory to generate simulated EXAFS spectra using FEFF for Fe-Ni bimetallic clusters on nitrogen doped carbon host.
  - Lower overpotential of 0.43V in Fe-Ni bimetallic clusters for oxygen reduction and evolution reactions was modeled using DFT and compared to 0.9 V for single-atom catalysts and 0.52 V for Pt. *Published in: Small.*
- **Computational and experimental investigation of solid-state isomerism of azobenzene in Mg-CUK-1L MOF**
  - Density functional theory was utilized to predict the trans azobenzene in CUK-1L MOF that was isomerized from cis azobenzene in MOF experimentally.
  - Accurately predicted reversible photo-isomerism by calculating the dielectric response using BSE equations, demonstrating expertise in the excited-state properties of hybrid materials. *Published in: J. Am. Chem. Soc.*
- **Vanadium (III) acetylacetonate soluble electrocatalyst for ORR and OER lithium-air battery applications**
  - Molecular simulations using electronic structure methods in ORCA predicted enhanced stability of intermediate superoxide by 0.54 eV due to charge transfer from vanadium.
  - Charge transfer facilitated the conversion of superoxide to peroxide during oxygen reduction/evolution reaction in the vanadium-based electrocatalyst in lithium-air batteries. *Published in: Angewandte Chemie*
- **Metal chalcogenide hollow polar bipyramid prisms as efficient electrocatalytic sulfur hosts for Na-S batteries**

- Computational modeling using meta-GGA functionals were used to accurately represent the half-metal state of cobalt chalcogenides was performed on different sodium sulfide discharge products as the cathode for Na-S batteries.
- The calculated formation energies were 1-2eV stronger compared to graphene, molecular phase, and solid phase of sodium sulfide discharge products which resulted in a high catalytic activity due to magnetic moment decrease in cobalt from 1.08 to 0.6 μ_M. *Published in: Nature Communications.*

- **Sodium-Antimony-Telluride intermetallic for the anode-free metal battery**
  - Using cluster enumeration, a new vacancy-rich intermetallic phase dispersed in sodium metal (NST-Na) was predicted and verified using XRD that enables 100% depth-of-discharge in sodium metal batteries.
  - Sodium atomic and cluster binding energy on NST-Na material was 0.8 eV weaker than overbinding copper surface but 0.2 eV stronger than underbinding pure sodium surface and chalcogenides which explained the enhanced performance of NST-Na compared to Na metal and Na_2Te or Na_3Sb. *Published in: Advanced Materials.*
- **Computational and experimental investigation of low valent metal ions as MOF pillars for C2 gas adsorption**
  - PCM-102 organophosphine MOF with pairs of offset trans-oriented P(III) donors were first synthesized and post-processed with metal salts to generate P_2-M solid-state complexes.
  - The Ag(I) PCM-102 MOF demonstrated an unusual strong binding to C2 gas with binding energy of 150% higher for C_2H_2 compared to C_2H_4, which was explained by 10-15% higher charge on C2 atoms in C_2H_2 from MOF ring structure. *Published in: J. Am. Chem. Soc.*

Indian Institute of Technology, Varanasi — ***Varanasi, India***
Integrated Master's Degrees — 2017-2018

- **Self-assembled polymeric nanofluid for biomedical membrane:** Siloxane-gold nanoparticle sol and polyindole-gold nanoparticle sol were synthesized and mixed together to produce self-assembled polymeric nanofluid for membrane casting. The membrane was tested for potentiometric ion sensor of both positive and negative ions. *Published in: MRS Communications.*

Technische Universität Darmstadt — ***Darmstadt, Germany***
DAAD Summer Scholar. — 2016

- **Simulating thermal resistance effects of solid-liquid interface on evaporation:** Solid-liquid interface Kapitza resistance's role on evaporation rate on a heated surface was studied using multiscale modeling. The interatomic potential was characterized by modeling the experimental wetting behavior through work of adhesion and thermal conductance of solid-liquid interfaces. Finally, the evaporation heat flux at the three phase contact line was calculated to understand the evaporation of droplets. *Published in: Langmuir.*

Academic Qualifications

University of Texas at Austin, Austin, TX — *Graduation:* May 2023
Ph.D. candidate in Chemistry, College of Natural Sciences — GPA: 4.0

Indian Institute of Technology, (BHU), Varanasi, India — *Graduation*: May 2018
Industrial Chemistry, 5-Year Integrated Master's Degree — GPA: 9.22