Dr. Sai VamsiKrishna Isukapalli

Computational Scientist | Molecular Simulation | Scientific ML | Materials Discovery

V.Isukapalli@lmu.de | Munich, Germany | Open to EU/UK/India roles

LinkedIn | Google Scholar| Git-Hub

PROFESSIONAL SUMMARY

Computational scientist with 8+ years of experience across ab initio molecular dynamics (AIMD), quantum chemistry, nonadiabatic dynamics, and scientific Python workflows. Current work at LMU Munich focuses on long-timescale AIMD of excess proton transport in water, large-scale trajectory analysis, and generation of DFT-quality energy/force datasets for message-passing ML interatomic potentials (MACE framework). Seeking materials-discovery and scientific-ML roles where simulation, data generation, and workflow engineering can accelerate R&D.

CORE STRENGTHS

Ab initio MD for condensed-phase systems, Nonadiabatic Excited-state dynamics to study ultrafast photophysics	DFT-quality dataset generation for ML interatomic potentials
Python analysis pipelines for large trajectories	HPC workflows, model validation, and scientific benchmarking

PROFESSIONAL EXPERIENCE

Postdoctoral Researcher — Theoretical Chemistry, LMU Munich Feb 2023 – Present | Munich, Germany

- Executed 250 ps AIMD of protonated liquid water in CP2K on national HPC systems, generating ~500k frames of DFT-quality trajectory data for structural and dynamical analysis.
- Built modular Python workflows for streaming multi-GB XYZ trajectories and extracting proton-sharing coordinates, RDFs, coordination metrics, and proton-transfer events.
- Generated energy/force datasets for a PaiNN/SchNetPack-style ML interatomic potential and supported dataset splitting, loss monitoring, hyperparameter tuning, and validation MD.
- Benchmarked simulation outputs against experiment and path-integral MD literature, with emphasis on proton transport observables and nuclear quantum effects.

Doctoral Researcher — Quantum Chemistry & Nonadiabatic Dynamics, IISER Thiruvananthapuram Aug 2018 – Feb 2023 | India

- Computed excited-state potential-energy surfaces and electronic couplings for organic chromophores using EOM-CCSD, MS-CASPT2, CASSCF, and TD-DFT workflows.
- Performed quantum-dynamics simulations with MCTDH and SHARC to quantify intersystem crossing, internal conversion, and time-resolved spectral signatures.
- Published peer-reviewed work and co-supervised Bachelor/Master students on computational chemistry projects and reproducible analysis workflows.

SELECTED TECHNICAL PROJECT

AIMD-to-MLIP Pipeline for Aqueous Proton Transport | CP2K, Python, PyTorch, MACE

- Prepared 497k DFT-quality energy/force snapshots from long-timescale AIMD as training data for a message-passing MLIP
- Developed reusable analysis code for proton-transfer event detection and condensed-phase structural descriptors, designed for large trajectory files and rapid validation loops.

EDUCATION

PhD, Computational Chemistry — IISER Thiruvananthapuram, India (awarded 2023)

Integrated M.Sc. (Hons.) Chemistry — BITS Pilani, India (2017)

B.E. (Hons.) Mechanical Engineering — BITS Pilani, India (2017)

TOOLS & METHODS

Quantum Chemistry: CP2K, ORCA, Gaussian, MOLPRO, TURBOMOLE, SHARC, MCTDH

Programming: Python, MATLAB, Bash, LaTeX

ML / Workflow: PyTorch, MACE, SchNetPack/PaiNN, HPC, SLURM, TensorBoard