Sarath Menon

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Profile

Computational materials scientist and software developer building AI for materials discovery, with 5+ years designing and applying machine learning interatomic potentials (MLIPs). Develop infrastructure for MLIPs (ACE, GRACE) in JAX and TensorFlow at ACEworks GmbH, and lead the Atomistic Simulation of Thermodynamic Properties group at ICAMS, Ruhr-University Bochum. Co-author on the foundational atomic cluster expansion (ACE/PACE) papers, developer of open-source tooling (calphy, pyscal, atomRDF, tools4RDF), and topical editor at the Journal of Open Source Software.

Skills

AI / ML: MLIPs, Graph Atomic Cluster Expansion (GRACE), atomic cluster expansion (ACE/PACE), JAX, TensorFlow, MLIP design, training, fine-tuning, parameterization, optimization, and benchmarking.

Atomistic simulation: LAMMPS (CUDA-accelerated builds on NVIDIA GPUs), VASP, Quantum Espresso, molecular dynamics, ab-initio datasets generation, free-energy methods.

Workflows & data: pyiron, automated MLIP to phase diagram workflows, knowledge graphs / RDF, reproducible research infrastructure (NFDI-MatWerk).

Programming: Python, C++, Bash.

Languages: English (fluent), German (B1), Spanish (A2), Malayalam (native).

Experience

Research Group Leader, Atomistic Simulation of Thermodynamic Properties — Mar 2025 – present
ICAMS, Ruhr-Universität Bochum

- Lead group research on thermodynamic properties through MLIPs with the aim of materials discovery at finite temperatures and automated phase diagram calculation.
- Direct method, software, and infrastructure development; supervise group members across training dataset generation, parameterization, and thermodynamic property workflows.

Software Developer — Jan 2025 – present
ACEworks GmbH, Bochum

- Develop infrastructure for foundational MLIPs including the deep learning-based GRACE and ACE-family MLIPs in JAX and TensorFlow for clients.
- Build customer-facing analysis, benchmarking, and workflow tooling.

Postdoctoral Research Assistant, Computational Materials Design — Feb 2022 – Mar 2025
Max Planck Institute for Sustainable Materials, Düsseldorf

- Methods and software for phase diagram calculation from atomistic simulations and MLIPs.
- Built reproducible computational workflows, software, and ontologies for the NFDI-MatWerk research data consortium.

Research Assistant — Oct 2020 – Feb 2022
Interdisciplinary Center for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum

- Developed automated benchmarking and validation pipelines for the atomic cluster expansion (ACE) MLIP family across structural, elastic, and thermodynamic properties.

Selected Publications

- **Menon, S.**; Guzmán, A.A.; Waseda, O.; Sandfeld, S.; Hickel, T. tools4RDF: a Python toolkit for working with RDF data. *J. Open Source Softw.* **2026**, 11, 9482.
- **Menon, S.**; Lysogorskiy, Y.; Knoll, A.L.M.; Leimeroth, N.; Poul, M.; Qamar, M.; Janssen, J.; Mrovec, M.; Rohrer, J.; Albe, K.; Behler, J.; Drautz, R.; Neugebauer, J. From electrons to phase diagrams with machine learning potentials using pyiron based automated workflows. *npj Comput. Mater.* **2024**, 10, 261.
- Bochkarev, A.; Lysogorskiy, Y.; **Menon, S.**; Qamar, M.; Mrovec, M.; Drautz, R. Efficient parametrization of the atomic cluster expansion. *Phys. Rev. Mater.* **2022**, 6, 013804.
- Lysogorskiy, Y.; Oord, C.; Bochkarev, A.; **Menon, S.**; Rinaldi, M.; Hammerschmidt, T.; Mrovec, M.; Thompson, A.; Csányi, G.; Ortner, C.; Drautz, R. Performant implementation of the atomic cluster expansion (PACE) and application to copper and silicon. *npj Comput. Mater.* **2021**, 7, 97.
- **Menon, S.**; Lysogorskiy, Y.; Rogal, J.; Drautz, R. Automated free-energy calculation from atomistic simulations. *Phys. Rev. Mater.* **2021**, 5, 103801.
- **Menon, S.**; Diaz Leines, G.; Rogal, J. pyscal: a python module for structural analysis of atomic environments. *J. Open Source Softw.* **2019**, 4, 1824.

Full publication list: Google Scholar (h-index 8; 680+ citations).

Open-Source Software

calphy: automated free-energy and phase-diagram calculation github.com/ICAMS/calphy

- Python tool driving LAMMPS to compute free energies and assemble phase diagrams; integrates with pyiron and MLIP backends.

pyscal: structural analysis of atomic environments github.com/pyscal/pyscal

- C++/Python module for local environment descriptors used in MLIP training data preparation and validation.

atomRDF & tools4RDF: ontology-based simulation data infrastructure github.com/pyscal/atomRDF

- Semantic annotation of atomic structures and computational workflows; knowledge graphs of simulation data for FAIR/reproducible materials research; methodology in arXiv:2604.06230.
- Powers kg.fair-workflows.org – an interactive materials knowledge-graph portal with LLM-driven natural-language to SPARQL querying (agentic exploration of simulation data).

Education

Doctor of Engineering, Mechanical Engineering 2017 – 2021
Ruhr-Universität Bochum, Germany

- Thesis: *Nucleation and growth during solidification in metals and alloys* – atomistic study of nucleation in BCC metals and binary metal–semiconductor alloys using rare-event sampling.

M.Sc., Materials Science and Simulation 2015 – 2017
Ruhr-Universität Bochum, Germany

B.Tech., Mechanical Engineering 2008 – 2012
National Institute of Technology, Calicut, India

Outreach

Topical Editor, Physics & Engineering Mar 2024 – present
Journal of Open Source Software

Workshops & teaching 2018 – present

- Designed and delivered workshops at meetings of the German Physical Society and German Society for Materials Science; teaching assistance for Master's-level simulation courses.

References

- **Prof. Dr. Ralf Drautz**, ICAMS, Ruhr-Universität Bochum and ACEworks GmbH
- **Prof. Dr. Jörg Neugebauer**, Max Planck Institute for Sustainable Materials