Aditya Sundar Ph.D. Computational Materials Scientist

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- Computational materials scientist experienced in active machine learning and simulation for accelerated materials discovery.
- Research portfolio in batteries, alloys, semiconductors, molecules, and hydrogen storage.
- Demonstrated history of simulation-experiment collaboration; Authored 20+ papers, 10+ conferences, 1 patent application.
- Interested in engineering informatics−based solutions for energy storage & conversion, catalysis, and electronic materials.

Skills

Methods	First principles simulations, molecular dynamics, computational thermodynamics, monte carlo, machine learned interatomic potentials, high−throughput screening, automated workflows, bayesian optimization
Atomic Simulation	VASP, Quantum ESPRESSO, LAMMPS, ART Nouveau (Activation Relaxation Technique)
Materials Simulation	Thermo-Calc, Abaqus FEA
Computation & design	Python (NumPy, mpi4py, Jupyter, Dash, asyncio, OpenCV), Mathematica, Linux, HPC, LaTeX
Machine learning	Scikit, TensorFlow, Keras, Pytorch, Pandas
Informatics	Chemprop, RDKit, pymatgen, ASE, DeePMD, matminer
Experiment	X−ray diffraction
Applications	Solid−state batteries, hydrogen storage, high−entropy alloys, ionic transport, alloys, coatings, additive manufacturing

Work Experience

Oct 2023 – Present
Computational Materials Scientist, National Energy Technology Laboratory
Leidos Inc.

Aug 2022 – Oct 2023
Postdoctoral Researcher, Argonne National Laboratory
Molecular Materials Group, Materials Science Division

May 2021 – Aug 2021
Research Intern, Idaho National Laboratory
Computational Mechanics and Materials Department

Achievements

Patent ’MULTIFUNCTIONAL COATINGS FOR SOLID STATE ELECTROLYTE POWDERS’, Serial No. 18/514,980

Awards First place in the Michigan Materials Research Institute Symposium poster presentation, 2021

Education

Sept 2017 – Aug 2022
Ph.D., University of Michigan in Materials Science and Engineering
Thesis: *Modeling the structural and chemical stability of materials in reactive environments using multiscale methods*

Aug 2015 – July 2017
M.S., Cornell University in Materials Science and Engineering
Thesis: *The Structure and Chemistry of Epitaxial 2D Chalcogenides*

Aug 2011 – July 2015
B.Tech., Indian Institute of Technology Madras in Metallurgical and Materials Engineering
Thesis: *Printed Silver Lines in MIS Solar Cells*

Research Publications

Journal Articles

1 **Sundar**, **A.**, Kim, T., Lagunas, F., Mane, A. U., Eze, U. D., Tepavcevic, S., ... Connell, J. G. (n.d.). Computationally-guided development of sulfide solid electrolyte powder coatings for enhanced stability and performance of solid-state batteries. *Under Review at Joule*.

2 **Sundar**, **A.**, Park, J., Park, H. P., Lee, E., Kim, J. J., & Zapol, P. (n.d.). Bayesian optimization of computed average voltage in entropy-stabilized metal fluoride conversion cathodes and their synthesis. *In Press at Journal of Power Sources*.

3 Tan, X., Trehern, W., **Sundar**, **A.**, Wang, Y., San, S., Lu, T., ... Hu, S. (n.d.). Machine learning and high-throughput computational guided development of high temperature oxidation-resisting ni-co-cr-al-fe based high-entropy alloys. *Under Review at npj Computational Materials*.

4 **Sundar**, **A.**, Tan, X., Hu, S., & Gao, M. C. (2025). Calphad-based bayesian optimization to accelerate alloy discovery for high-temperature applications. *Journal of Materials Research*, 1–11. link.

5 Ercan, C., Mahmut, N. C., **Sundar**, **A.**, Eugene, M., Jianguo, Y., Xunxiang, H., & Kory, D. L. (2024). Hydrogen motion in stoichiometric yttrium dihydride at elevated temperatures. *Journal of Nuclear Materials*, *593*, 154972. link.

6 Jobes, D., Rubio-Ejchel, D., Lopez, L., Jenkins, W., **Sundar**, **A.**, Tandoc, C., ... Hu, Y.-J. et al. (2024). Computationally guided alloy design and microstructure-property relationships for non-equiatomic ti–zr–nb–ta–v–cr alloys with tensile ductility made by laser powder bed fusion. *Materials Science and Engineering: A*, *911*, 146922. link.

7 Kim, J. J., Kc, B., Park, H., **Sundar**, **A.**, Evmenenko, G., Buchholz, D. B., ... Klie, R. F. et al. (2024). Strain-driven surface reactivity in magnesium-ion battery cathodes. *Chemistry of Materials*, *36*(3), 1342–1351. link.

8 Kim, T., Hood, Z. D., **Sundar**, **A.**, Mane, A. U., Lagunas, F., Kumar, K., ... Elam, J. W. et al. (2024). Suppressing atmospheric degradation of sulfide-based solid electrolytes via ultrathin metal oxide layers. *ACS Materials Letters*, *6*(12), 5409–5417. link.

9 Park, J., Yang, Y., Park, H., **Sundar**, **A.**, Lee, S., Kinnibrugh, T. L., ... Klie, R. F. et al. (2024). Entropy-stabilized multication fluorides as a conversion-type cathode for li-ion batteries–impact of element selection. *ACS applied materials & interfaces*, *16*(42), 57151–57161. link.

10 **Sundar**, **A.**, Feinauer, A., Kinzer, B., Petrasch, J., Qi, L., & Bala Chandran, R. (2024). Thermodynamic, kinetic and mechanical modeling to evaluate co2-induced corrosion via oxidation and carburization in fe, ni alloys. *Corrosion Science*, *229*, 111850. link.

11 **Sundar**, **A.**, Yu, J., & Cinbiz, M. N. (2024). Effect of impurities on hydrogen defect stability and migration barrier in yttrium dihydride crystal. *International Journal of Hydrogen Energy*. link.

12 Hood, Z. D., Mane, A. U., **Sundar**, **A.**, Tepavcevic, S., Zapol, P., Eze, U. D., ... Elam, J. W. et al. (2023b). Multifunctional coatings on sulfide-based solid electrolyte powders with enhanced processability, stability, and performance for solid-state batteries. *Advanced Materials*, *35*(21), 2300673. link.

13 **Sundar**, **A.**, Ferron, D. B., Hu, Y.-J., & Qi, L. (2022). Automated hierarchical screening of refractory multicomponent alloys with high intrinsic ductility and surface passivation potency. *MRS Communications*, *12*(6), 1086–1095. link.

14 **Sundar**, **A.**, Huang, Y., Yu, J., & Cinbiz, M. N. (2022). The impacts of charge transfer, localization, and metallicity on hydrogen retention and transport capacity. *International Journal of Hydrogen Energy*. link.

15 **Sundar**, **A.**, Yu, J., Qi, L., & Cinbiz, M. N. (2022). High temperature stability and transport characteristics of hydrogen in alumina via multiscale computation. *International Journal of Hydrogen Energy*, *47*(75), 32345–32357. link.

16 Hu, Y., **Sundar**, **A.**, Ogata, S., & Qi, L. (2021). Screening of generalized stacking fault energies, surface energies and intrinsic ductile potency of refractory multicomponent alloys. *Acta Materialia*, *116800*. link.

17 **Sundar**, **A.**, Chen, G., & Qi, L. (2021b). Substitutional adsorptions of chloride at grain boundary sites on hydroxylated alumina surfaces initialize localized corrosion. *npj Materials Degradation*, *5*. link.

18 **Sundar**, **A.**, & Qi, L. (2021). Stability of native point defects in Al_2O_3 under aqueous electrochemical conditions. *Journal of Applied Electrochemistry*. link.

19 Lu, H., Reese, C., Jeon, S., **Sundar**, **A.**, Fan, Y., Rizzi, E., ... Goldman, R. (2020). Mechanisms of GaN quantum dot formation during nitridation of Ga droplets. *Applied Physics Letters*, *116*(6), 062107. link.

20 Li, W., Nomoto, K., **Sundar**, **A.**, Lee, K., Zhu, M., Hu, Z., … Gao, X. et al. (2019). Realization of GaN PolarMOS using selective-area regrowth by MBE and its breakdown mechanisms. *Japanese Journal of Applied Physics*, *58*(SC), SCCD15. link.

21 Vishwanath, S., **Sundar**, **A.**, Liu, X., Azcatl, A., Lochocki, E., Woll, A. R., … Peng, X. et al. (2018). MBE growth of few-layer 2H-$MoTe_2$ on 3D substrates. *Journal of Crystal Growth*, *482*, 61–69. link.

Conference Proceedings

1 Hu, S., Tan, X., Lu, T., **Sundar**, **A.**, Wang, Y., San, S., & Gao, M. (2025). Development of nicofecral based high entropy alloys for hydrogen fueled turbine system. In *2025 TMS Annual Meeting & Exhibition*, Las Vegas, USA.

2 Oleksak, R., Trehern, W., **Sundar**, **A.**, Chong, L., Wenzlick, M., Rozman, K., … Gao, M. (2025). Predicting alloy oxidation resistance using physics-informed machine learning. In *2025 TMS Annual Meeting & Exhibition*, Las Vegas, USA.

3 Tan, X., Trehern, W., **Sundar**, **A.**, Wang, Y., San, S., Lu, T., … Hu, S. (2025). Machine learning and high-throughput computations guided development of high temperature oxidation-resisting ni-co-cr-al-fe high-entropy alloys. In *2025 TMS Annual Meeting & Exhibition*, Las Vegas, USA.

4 **Sundar**, **A.**, Chen, G., & Qi, L. (2024). Simulations of chloride on hydroxylated passive oxide surfaces related to localized corrosion initialization. In *2024 TMS Annual Meeting & Exhibition*, Orlando, USA.

5 Trehern, W., **Sundar**, **A.**, Chong, L., Oleksak, R., Wenzlick, M., Rozman, K., … Gao, M. (2024). Predicting oxidation behavior of ni-based superalloys with physics-informed machine learning. In *MS&T24: Materials Science Technology*, Pittsburgh, USA.

6 Hood, Z. D., Mane, A. U., **Sundar**, **A.**, Tepavcevic, S., Zapol, P., Eze, U. D., … Elam, J. W. et al. (2023a). Multifunctional coatings on sulfide-based solid electrolyte powders with enhanced processability, stability and performance for solid-state batteries. In *2023 MRS Fall Meeting & Exhibit*, Boston, USA.

7 Qi, L., **Sundar**, **A.**, & Hu, Y.-J. (2023). Automated hierarchical screening of refractory multicomponent alloys with high intrinsic ductility and surface passivation potency. In *7th world congress on integrated computational materials engineering (icme 2023)*.

8 **Sundar**, **A.**, Bugallo-Ferron, D., Hu, Y.-J., & Qi, L. (2022). Computational search for bcc refractory alloys with enhanced strength, ductility and corrosion resistance. In *2022 mrs spring meeting & exhibit*, Honolulu, USA.

9 **Sundar**, **A.**, Chen, G., & Qi, L. (2022). Modeling of chloride effect on localized corrosion initiation at grain boundary sites of passive oxide surfaces. In *2022 mrs spring meeting & exhibit*, Honolulu, USA.

10 Hu, Y.-J., **Sundar**, **A.**, Chen, G., & Qi, L. (2021). Title: Screening of generalized stacking fault energies, surface energies and intrinsic ductile potency of refractory multicomponent alloys. In *The Minerals, Metals & Materials Society 2021 Annual Meeting & Exhibition*, Orlando, USA.

11 Kinzer, B., **Sundar**, **A.**, & Bala Chandran, R. (2021). Oxide dispersion particle clustering using phase field modelling in nickel-based superalloys. In *2021 mrs spring meeting & exhibit*, Phoenix, USA.

12 **Sundar**, **A.**, Chen, G., & Qi, L. (2021a). Electronic structure mechanisms to explain the onset of Cl-induced localised corrosion in Al_2O_3. In *The Minerals, Metals & Materials Society 2021 Annual Meeting & Exhibition*, Orlando, USA.

13 **Sundar**, **A.**, Kinzer, B., & Bala Chandran, R. (2021). Oxidation and carburization behavior of iron- and nickel-based alloys in supercritical CO_2 environments. In *2021 MRS Spring Meeting & Exhibit*, Phoenix, USA.

14 **Sundar**, **A.**, & Qi, L. (2019). Electric field dependent ionic transport in passive corundum Al_2O_3 from DFT: Application to localized corrosion. In *2019 MRS Fall Meeting & Exhibit*, Boston, USA.

Research Experience

National Energy Technology Laboratory — Oct 2023–present
Computational Materials Scientist

High-throughput computation for Additive Manufacturing of High Temperature Alloys

- Developed parallel TC-Python workflows to compute thermophysical properties of ∼100k alloys using CALPHAD.
- Recommended alloys using multi−objective Bayesian Optimization to minimize CTE & brittle phase content.
- Developing ML models for vacancy thermodynamics in multi−component Ni alloys

Research Experience (continued)

Argonne National Laboratory, Lemont, USA — Aug 2022–Oct 2023
Postdoctoral Researcher, Materials Science Division

Bayesian Optimization of Voltage in High-Entropy Conversion Cathodes with Earth-Abundant Elements

- Implemented Bayesian optimization algorithm to screen high voltage cathodes by sampling <2% of the search space
- Discovered Ni, Co-free non-equimolar chemistries with ∼28% improved voltage over conventional equimolar fluorides
- Experimental validation shows room temperature synthesizability, phase purity, and improved cell voltages

Active Learning Workflows to develop Neural Network Force Fields for Solid-State Batteries

- Developed neural network-based force fields for Li-conductivity in solid electrolytes (speed ×6500, accuracy ∼91%)
- Achieved within ∼10% match to experimental measurements of Li diffusivity and energy barrier
- Setup computational screening protocols and identified multifunctional oxide coatings to improve battery performance
- Experimental validation shows improved chemical stability and transport properties arising from conformal coatings

Data Pipeline for Molecule Discovery in Redox Flow Batteries

- Discovered Benzothiadiazole−derivative small molecules that improve the cell voltage of redox−flow batteries
- Built gradient boosting regressors & neural networks to predict the reduction potential of 6k molecules (RDkit, scipy)
- Built graph neural networks tuned using Bayesian optimization with 10% lower errors (chemprop, Hyperopt, speed ×100)
- Containerized web app (Dash, Plotly) using Docker and deployed on AWS ECS to display model results
- Designed single and multi−target ML models to predict the emission & absorption wavelengths of molecules in OLEDs

University of Michigan, Ann Arbor, USA — Sep 2017–July 2022
Department of Materials Science and Engineering

High-Throughput Discovery of Refractory Alloys with Enhanced Manufacturability

- Automated the acquisition of high fidelity data from ∼3k DFT calculations on HPC systems, using Python/Bash scripting.
- Built cross-validated Random Forest Regressors by feature engineering a sparse 130-entry dataset (Scikit, $R^2 > 0.93$)
- Deployed the model on HPC platforms (mpi4py, numpy) to explore $\sim 10^7$ alloys; improved efficiency ×10000.
- Developed a parallel Python code (numpy, ThermoCalc-Python API) to compute ∼600k phase diagrams (speed ×20).
- Discovered high-entropy alloys with enhanced manufacturability and corrosion resistance, built interactive dashboards
- Model predictions validated by additively manufactured alloys demonstrating high ductility

Multiscale Simulation of Oxide Coatings for High Temperature Energy Applications

- Formulated empirical models for CO2-induced corrosion in metals by combining experimental and CALPHAD databases
- Automated FEA simulations and showed enhanced residual stresses in alloy-coating interfaces due to carburization
- Recommended Ni-rich Haynes 214 over Fe-rich Incoloy MA956 due to reduced carburization between 600-900°C

Ab initio modeling of surface stability and reactivity in semiconductor-electrolyte interfaces

- Combined classical force fields and Activation Relaxation Technique simulations for efficient sampling.
- Investigated the dynamical stability and reactivity of Al_2O_3-electrolyte interfaces using computational electrochemistry
- Proposed thermodynamic solvation models to explain sustained catalytic Al_2O_3 dissolution in chloride electrolytes.

Idaho National Laboratory, Idaho Falls, USA — May 2021–Aug 2021
Research Internship, Computational Mechanics and Materials organization

- Built active learned Gaussian approximation potentials using density-based clustering of molecular dynamics datasets.
- Achieved ×350 simulation speeds; within 8% agreement between simulated and experimental proton diffusivity in Al_2O_3.
- Proposed alloying elements to improve hydrogen storage in YH_2 (nuclear micro-reactor candidate), using DFT.
- Gained experience with GPU accelerated neural networks applied in reactor engineering and image analysis.

Research Experience (continued)

Cornell University, Ithaca, USA
Department of Materials Science and Engineering
Aug 2015–July 2017

Structural, chemical and electronic characterization of MBE grown 2D materials

- Confirmed ∼44% Te alloying in MBE $MoSe_xTe_{2-x}$ on CaF_2 and GaAs substrates; by XRD, Raman, XPS, TEM, EXAFS.
- Compositional variation of bandgap and excitonic states shown by absorption spectroscopy.
- Imaged crystallographic orientation, twinning, and mosaicity in ultrathin 2D heterostructures (graphene-TMDs).
- Developed Mathematica scripts to parse, analyze and visualize large datasets obtained from synchrotron experiments.
- Identified highly conductive leakage paths along MBE regrown interfaces using conductive AFM.

Service

Reviewer

Journal of Materials Research, Applied Materials Today, The Journal of Physical Chemistry, Journal of Non-Crystalline Solids, Journal of Computing and Information Science in Engineering, Computational Materials Science, Engineering Applications of Artificial Intelligence.