Aditya Sundar, Ph.D student, University of Michigan

adisun@umich.edu +1 734-450-1424

Interested in automated materials discovery for applications in energy and electronics

Education

2017 – 2022 **Ph.D., University of Michigan** in Materials Science and Engineering CGPA: 3.93/4.00
Thesis: *Modelling the structural and chemical stability of materials in extreme environments*
Certificate: Computational Discovery and Engineering
Advisor: Liang Qi

2015 – 2017 **M.S., Cornell University** in Materials Science and Engineering CGPA: 3.90/4.00
Thesis: *The Structure and Chemistry of Epitaxial 2D Chalcogenides*
Advisor: Huili Grace Xing

2011 – 2015 **B.Tech., Indian Institute of Technology Madras** CGPA: 8.66/10.00
in Metallurgical and Materials Engineering
Thesis: *Printed Silver Lines in MIS Solar Cells*
Advisor: Parasuraman Swaminathan
Minor degree: Management studies

Experience

Summer 2021 **Idaho National Laboratory,** Idaho Falls, USA
Research Internship, Computational Mechanics and Materials organisation

- Screened solid-state alkali, alkaline earth and transition metal hydrides with high hydrogen conduction/retention by analyzing correlations between electronic structure and defect stability.
- Recommended the use of metallic YH_2 as a neutron moderator over other transition metal hydrides, due to extended hydrogen retention capacity arising from strong charge localization.
- Recommended crystalline Al_2O_3 as a suitable cladding oxide with poor hydrogen permeability arising from localized proton trap states, from molecular statics and ab initio molecular dynamics simulations.
- Accelerated MD simulations of H diffusion in amorphous Al_2O_3 by training machine learned Gaussian approximation potentials; implemented density-based clustering of computational chemistry datasets.
- Developed MPI/Python based monte carlo simulations to quantify hydrogen stability and retention in different candidate materials, including the use of open-source materials databases and libraries.
- Gained experience with neural network and GPU acceleration methods applied to solve problems in reactor engineering and image analysis.

Skills

Applications	Ionic transport, semiconductor-electrolyte interfaces, surface passivation, catalysis, solid state hydrides, refractory alloys
Methods	First principles simulations, molecular dynamics, kinetic monte carlo, computational thermodynamics, force field, high throughput screening, automated workflows
Atomic Simulation	VASP, Quantum ESPRESSO, LAMMPS, ART Nouveau (Activation Relaxation Technique)
Materials Simulation	Thermo-Calc
Computation & design	Python (NumPy, mpi4py), Mathematica, Linux, HPC, LaTeX
Data Analysis	Machine learning & statistical regression (Scikit, Pandas, OpenCV, Jupyter, R), pymatgen
Experiment	XRD, XPS, Raman, Conductive-AFM

Research Publications

Manuscripts in Preparation

1 **Sundar**, **A.**, & Qi, L. (n.d.). Automated hierarchical screening of BCC refractory alloys with high intrinsic strength, ductility and corrosion resistance using DFT-statistical-CALPHAD methods.

2 **Sundar**, **A.**, Yu, J., & Cinbiz, M. (n.d.). Revealing slow diffusion of protonic interstitials in alumina using machine learned accelerated molecular dynamics.

Journal Articles

1 **Sundar**, **A.**, Huang, Y., Yu, J., & Cinbiz, M. (n.d.). Charge transfer, localisation and metallicity lead to large hydrogen retention capacity in transition metal dihydrides: YH_2 and ZrH_2. *Submitted*.

2 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.

3 **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.

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

5 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.

6 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.

7 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, 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.

2 **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.

3 **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.

4 **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

2020 – 2022 **Hierarchical high throughput screening of high entropy refractory alloys.**

- Developed atomistic models to compute the average room temperature strength and ductility of high entropy refractory alloys using DFT-SQS methods.
- Devised random forest and gradient boosted regression models for rapid strength and ductility prediction of $\sim 10^8$ multicomponent BCC alloys, using a sparse dataset with 150 systems (Scikit, Numpy, Pandas).
- Automated CALPHAD based computational workflows using the TC-Python package & custom parallelised Python codes, for the high-throughput calculation of $\sim$600,000 refractory alloy phase diagrams.
- Identified promising BCC alloy compositions with high room temperature ductility and corrosion resistance by surface passivation.

Research (continued)

2018 – 2021 **Ab initio modelling of surface stability and reactivity in semiconductors**

- Validated the Point Defect Model by designing DFT based thermodynamic models to investigate the dynamical stability and reactivity of Al_2O_3 surfaces in halide electrolytes.
- Analyzed root causes driving surface sensitive Cl adsorption on Al_2O_3 and surface reaction mechanisms; from static and dynamic molecular simulations in standard aqueous conditions.
- Proposed thermodynamic solvation models to explain experimental observations of sustained catalytic Al_2O_3 dissolution in Cl containing elcetrolytes.
- Investigated the root causes that enhance silver atom adsorption at defect sites on wurtzite ZnO surfaces

2020 – 2021 **Alloy selection for high temperature heat exchanger materials, in supercritical CO_2**

- Developed CALPHAD based empirical thermokinetic models to study oxidation-carburization of Fe and Ni alloys in supercritical CO_2, up to 1000 °C and 200 bar pressure.
- Empirical mass balance formalism can be used to compute the carbon activity at the metal-oxide interface, parametrized using real experimental data.
- Recommended the use of Ni based Haynes 214 due to better carburization resistance (limited brittle carbide precipitation) compared to Fe based Incoloy MA 956, from 1D diffusion-reaction simulations.

2019 – 2019 **Thermodynamic model for GaN quantum dot formation**

- Provided ab initio results to explain surface coverage dependent GaN quantum dot formation on Si. Results used to interpret morphological characteristics of MBE grown GaN quantum dots.
- Designed and calculated adsorption thermodynamics of Ga atoms to explain QD size distribution on oxidised and nitrided Si(100)-2×2 reconstructed surfaces.

2015 – 2017 **Structural, chemical and electronic characterization of MBE grown 2D materials**

- Confirmed up to 44% Te alloying in MBE $MoSe_xTe_{2-x}$ on CaF_2 and GaAs substrates; by XRD, Raman, XPS, TEM and EXAFS examinations. Compositional variation of bandgap and excitonic states shown by absorption spectroscopy.
- Imaged crystallographic orientation, twinning and mosaicity in ultrathin 2D heterostructures (graphene-transition metal dichalcogenides) by synchrotron measurements.
- Developed Mathematica scripts to parse, analyze and visualize large datasets obtained from synchrotron based diffraction and spectroscopy experiments.
- Identified highly conductive leakage paths along MBE regrown interfaces by correlating topography and current area maps, to explain limited reverse breakdown voltage.

Projects

Fall 2021 **Designed a MPI/Python automation script to efficiently select ab initio datasets to train Gaussian Approximation Potential interatomic potentials, and accelerate MD simulations.**

Fall 2020 **Computer Vision**
Implemented a OpenCV and scikit based fruit-sorting algorithm using blob detection and superpixel image segmentation methods; to sort fresh and rotten fruits.

Winter 2020 **Data-Driven Materials Design and Genomics**
Automated data retrieval using the Materials Project API; engineered features to model correlations between structural properties and Li ion conductivity.

Projects (continued)

Fall 2019 — Time Series Modeling, Forecasting, Analysis
Implemented seasonal ARIMA models in R to predict AirBnb locations based on local crime rate.

Winter 2018 — Kinetic Monte Carlo simulations of crystal growth
Developed 2D codes and visualisations in Mathematica to simulate the epitaxial growth of zinc blende GaAs. Surface diffusion energies from molecular dynamics calculations were used to evaluate temperature dependent point defects and surface morphologies.

Mentoring and Leadership

2019 – 2021

- Guided and trained Master's degree student in the design and implementation of first principles calculations using VASP. Research topics included (1) surface stability of passive oxides and (2) electronic structure origin of Cl-induced depassivation.
- Mentored research projects for 3 undergraduate students in the (1) design of ab initio calculations, (2) implementation of ab initio calculations using Quantum Espresso and (3) analysis of results. Topics covered included (1) thermodynamic stability of semiconductor polymorphs and (2) electronic stability of point defects in crystal semiconductors.
- Lab group server & website operations: http://cms.engin.umich.edu/
- Vice President, SPIC MACAY (Society for the Promotion of Indian Classical Music And Culture Amongst Youth), University of Michigan chapter. Led a team of 10-15 students in the organisation of biannual musical concerts in the university. Responsible for securing grants and event logistics.

Fall 2021 — Graduate Student Instructor for senior materials science course. Familiarised students with atomic modelling and visualisation software (VESTA).

Fall 2018 — Graduate Student Instructor for undergraduate materials science course. Led weekly discussions and office hours, and designed problem sets and demonstrations for a class of 30 undergraduate students.

References

Prof. Liang Qi
Materials Science and Engineering
University of Michigan, Ann Arbor, MI, 48109
qiliang@umich.edu
+1 734 615 8086

Dr. Jianguo Yu
Staff Scientist, Computational Mechanics and Materials Organization
Idaho National Laboratory, Idaho Falls, ID, 83415
jianguo.yu@inl.gov

Dr. Mahmut Cinbiz
Staff Scientist, Material and Fuels Complex
Idaho National Laboratory, Idaho Falls, ID, 83415
Mahmut.Cinbiz@inl.gov