Aditya Sundar, Ph.D student, University of Michigan, USA

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Interested in developing data-driven computational models and workflows for materials discovery

Education

2017 – 2022 **Ph.D., University of Michigan** in Materials Science and Engineering — CGPA: 3.93/4.00
Thesis: *Modeling the structural and chemical stability of materials in reactive environments using multiscale methods*
Certificate: Computational Discovery and Engineering

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*

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*
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 for hydrogen storage applications by analyzing correlations between electronic structure and defect stability.
- Recommended the use of early transition-metal hydrides YH_2 and ZrH_2 as solid-state hydrogen storage materials due to high retention capacity arising from charge localization.
- Developed active machine learned Gaussian approximation potentials to model the performance of alumina polymorphs as H permeation barriers; using density-based clustering of AIMD datasets.
- Achieved $\times$350 improvement in MD simulation speeds (for few 100 atoms) and within 7% agreement in H diffusivity between machine learned MD and ab initio MD data.
- Provided a mechanistic understanding of high temperature stability and transport mechanisms of H species in Al_2O_3 polymorphs; within 8% agreement between simulated and experimental diffusivity.
- 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 (DNN, CNN) and GPU acceleration methods applied to solve problems in reactor engineering and image analysis.

Skills

Applications	Molecular adsorption, hydrogen storage, catalysis, reaction pathways, ionic transport, semiconductor-electrolyte interfaces, surface passivation & coatings
Methods	First principles simulations, molecular dynamics, computational electrochemistry, 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, Jupyter, OpenCV), Mathematica, Linux, HPC, LaTeX
Data Analysis	Machine learning & regression (Scikit, TensorFlow, Pandas, R), pymatgen, ASE, DScribe
Experiment	Diffraction, spectroscopy

Research Publications

Manuscripts in Preparation

1 **Sundar**, **A.**, Ferron, D. B., Hu, Y.-J., & Qi, L. (n.d.). Automated hierarchical screening of refractory multicomponent alloys with high intrinsic ductility and corrosion resistance. *In Review, MRS Communications*.

2 **Sundar**, **A.**, Yu, J., Qi, L., & Cinbiz, M. (n.d.). Accelerated molecular dynamics using machine learned force fields reveals slow diffusion of protonic interstitials in alumina. *Submitted, ACS Chemistry of Materials*.

Journal Articles

1 **Sundar**, **A.**, Huang, Y., Cinbiz, M., & Yu, J. (n.d.). The impacts of charge transfer, localization, and metallicity on hydrogen retention and transport capacity. *In Press, International Journal of Hydrogen Energy*.

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 **Sundar**, **A.**, & Qi, L. (2022a). Computational search for bcc refractory alloys with enhanced strength, ductility and corrosion resistance. In *2022 mrs spring meeting & exhibit*, Honolulu, USA.

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

3 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.

4 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.

5 **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.

6 **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.

7 **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 of metal surface and metal-metal interface structures to compute the room temperature strength and ductility of multicomponent refractory alloys using DFT-SQS methods
- Designed Python/Bash scripts to automate the preparation, submission and analysis of $\sim$3000 DFT calculations on HPC systems.
- Devised random forest and gradient boosted regression models for rapid strength and ductility prediction of $\sim 10^7$ multicomponent BCC alloys, using a sparse dataset with 130 systems (Scikit, Numpy, Pandas).
- Automated CALPHAD based computational workflows using the TC-Python API (with customized parallel scripts) for the high-throughput calculation of $\sim$600,000 refractory alloy phase diagrams.
- Identified promising BCC alloy compositions with enhanced room temperature ductility and high temperature corrosion resistance by surface passivation; validated properties using DFT calculations.
- Designed deep neural networks in TensorFlow (with GPU support) for the accurate prediction of BCC mass fraction in multicomponent alloys.

2018 – 2021 **Ab initio modelling of surface stability and reactivity in semiconductor-electrolyte interfaces**

- Validated the Point Defect Model by designing DFT based computational electrochemistry models to investigate the dynamical stability and reactivity of Al_2O_3 surfaces in halide electrolytes.
- Designed a 3-step protocol to generate point defect phase diagrams for oxides in electrochemical conditions, by combining classical force fields and Activation Relaxation Technique simulations.
- Developed mechanistic models to analyze the root causes driving surface sensitive Cl adsorption on Al_2O_3 and surface reaction mechanisms; from molecular statics and dynamics simulations in standard electrochemical conditions.
- Proposed ab initio paramatrized thermodynamic solvation models to explain experimental observations of sustained catalytic Al_2O_3 dissolution in Cl containing elcetrolytes.

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 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.

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 4 students (1 graduate + 3 undergraduate) in the design, implementation and analysis of first principles calculations using VASP and Quantum Espresso. Research topics included (1) surface stability of passive oxides and (2) electronic structure origin of Cl-induced depassivation, (3) thermodynamic stability of semiconductor polymorphs and (4) 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.