Aditya Sundar, Ph.D student, University of Michigan

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Interested in applying computational chemistry methods to accelerate material discovery for energy applications

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

- Implemented atomistic simulations to guide the selection of materials with large hydrogen retention capacity, for application as next-generation nuclear microreactor components
- 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 pure YH_2 as a neutron moderator due to extended hydrogen retention capacity at high temperatures, compared to alloyed hydrides
- Recommended Al_2O_3 as a suitable cladding oxide with poor hydrogen permeability, from molecular dynamics simulations
- Setup automation scripts for high throughput HPC calculations and Python workflows using Jupyter for efficient data analysis and visualization.
- 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.

Skills

Applications	Electrochemistry, surfaces & coatings, permeation barriers, alloy design
Methods	Electronic structure, molecular dynamics, monte carlo, potential energy landscape, computational thermodynamics, spectroscopy
Atomic Simulation	VASP, Quantum ESPRESSO, LAMMPS, ART Nouveau (Activation Relaxation Technique)
Materials Simulation	Thermo-Calc
Computation & design	Python, Mathematica, LaTeX, Linux, HPC
Data Analysis	Machine learning (NumPy, Scikit, openCV, Jupyter, R), mpi4py, pymatgen
Experiments	XRD, XPS, Raman, Conductive-AFM

Research Publications

Manuscripts in Preparation

1 **Sundar**, **A.**, Yu, J., & Cinbiz, M. (n.d.[a]). Charge transfer, localisation and metallicity lead to large hydrogen retention capacity in transition metal dihydrides: Yh_2 and zrh_2.

2 **Sundar**, **A.**, Yu, J., & Cinbiz, M. (n.d.[b]). Hydrogen stability and transport in al2o3 claddings.

Journal Articles

1 Vishwanath, S., **Sundar**, **A.**, Liu, X., Azcatl, A., Lochocki, E., Woll, A. R., ... Peng, X. et al. (2018). Mbe growth of few-layer 2h-mote2 on 3d substrates. *Journal of Crystal Growth*, *482*, 61–69. link.

2 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.

3 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.

4 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.

5 **Sundar**, **A.**, & Qi, L. (2021). Stability of native point defects in al2o3 under aqueous electrochemical conditions. *Journal of Applied Electrochemistry*. link.

6 **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.

Conference Proceedings

1 **Sundar**, **A.**, & Qi, L. (2019). Electric field dependent ionic transport in passive corundum al2o3 from dftapplication to localized corrosion. In *2019 mrs fall meeting & exhibit*, Boston, USA.

2 **Sundar**, **A.**, Chen, G., & Qi, L. (2021a). Electronic structure mechanisms to explain the onset of cl-induced localised corrosion in al2o3. 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 co2 environments. In *2021 mrs spring meeting & exhibit*, Phoenix, 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 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.

Research

2020 – 2022 **Screening high entropy refractory alloys for ICME guided additive manufacturing**

- Developed CALPHAD/DFT based machine learning models to compute room temperature strength and ductility of metallic alloys.
- Designed physics-based quantile regression models to predict properties of multicomponent refractories using a sparse dataset composed of $\sim$ 100 binary and ternary systems.
- Efficiently screened over 10^7 alloys by reducing calculation times from days to seconds, using customised MPI/Python scripts.
- Awarded best poster at Michigan Materials Research Institute symposium 2021.

Research (continued)

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

- Validated the Point Defect Model by designing thermodynamic models to investigate Al_2O_3 depassivation in halide electrolytes.
- Identified the root causes driving Cl adsorption at weak surface sites; from static and dynamic molecular simulations in standard aqueous conditions.
- Analyzed the root causes and surface sensitivity of Cl adsorption at weak surface sites on Al_2O_3; from static and dynamic molecular simulations in standard aqueous conditions.
- Analyzed the sensitivity of Cl adsorption to explain experimental observations of sustained catalytic Al_2O_3 dissolution.
- 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 thermokinetic models to study oxidation-carburization of Fe and Ni alloys in supercritical CO_2, up to 1000 °C and 200 bar pressure.
- Recommended the use of Ni based Haynes 214 due to better carburization resistance compared to Fe based Incoloy MA 956, from 1D diffusion-reaction simulations.
- Model explains larger severe carburization induced corrosion in Fe alloys, due to larger amounts of brittle carbide precipitation and carburization depths.

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 GAP 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.

Projects (continued)

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 a 2D code and Mathematica visualisations 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
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