Shu Huang

Curriculum Vitae – Modeling and Computational Science

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Research Interests

Computational materials science, machine learning applications in materials modeling, nuclear materials, multiferroic devices, and fusion energy research.

Education

2016–2022 **Ph.D. in Materials Science**, *University of California, Los Angeles*, Los Angeles, USA
Dissertation: *[Multi-Scale Modeling and Simulations for Materials Phenomena]*

2014–2016 **M.Sc. in Materials Engineering**, *University of Southern California*, Los Angeles, USA

2010–2014 **B.Sc. in Applied Physics**, *Hefei University of Technology*, Hefei, China

Work Experience & Projects

2022–Present **Software Engineer**, *Workday Inc.*, San Francisco Bay Area, USA

- **What-if Scenario Modeling & Simulation for Agile Business Planning**
  - Designed and implemented **What-if Scenario Modeling and Simulation**, leveraging **data analysis, modeling, and database development** to help businesses assess the impact of various course-correcting measures.
  - Integrated **analytics and reporting** features to generate **data-driven insights**, enabling organizations to visualize trends, identify opportunities, and mitigate risks.

2017–2022 **Research Assistant**, *Marian's Group, UCLA*, Los Angeles, USA

- **Machine Learning Modeling on Tungsten Oxidation**:
  - Developed databases, regression models (CNN, Random Forest, k-NN) to predict oxidation growth curves of Tungsten.
- **Kinetics Model of Multi-layer Tungsten Oxide**:
  - Developed kinetics models in Java to simulate interface front trajectories using the Stefan model and partial differential equations for diffusion.
  - Conducted large-scale simulations on a distributed computing system to analyze the oxidation process of tungsten, a critical material for fusion reactor chambers.
- **Finite Element Methods on Multiferroic Devices**:
  - Used FEM in C++ and COMSOL to analyze mechanical response in multi-ferroic materials consisting of a CFO and PZT.
  - Revealed that shear coupling at the interface significantly enhances the deformation in the piezoelectric effect, demonstrating the material's strong potential as a promising candidate for piezoelectric devices.
- **Modeling & Simulation of Fusion Irradiation Damage**:
  - Derived analytical expressions for coagulation rates and absorption rates at sinks for species generated by irradiation damage, moving along 1D trajectories.
  - The analytical derivations were validated through Kinetic Monte Carlo simulations, demonstrating a more precise estimation compared to traditional reaction rate calculations.

2017–2020 **Teaching Assistant**, *UCLA*, Los Angeles, USA

- **MSE 270 Computer Simulations of Materials**: Conducted instructional sessions and led discussions on computational modeling methods, including basic statistical mechanics, classical molecular dynamics, and Monte Carlo methods. Assisted in designing, running, and analyzing more than 15 computer simulations of materials.

2016 **Engineering Manager**, *Alpha Ring LLC*, Los Angeles, USA

- Developed fusion reactor systems, vacuum cooling mechanisms.
- Optimized power input-output efficiency using LabVIEW, improving energy output ratio from 2.0 to 3.5.

Workshops & Summer Schools

Oct, 2019 **International Conference on Fusion Reactor Materials**, *University of California, Los Angeles*

Jul, 2019 **Modeling Experimentation Validation Summer School**, *Oak Ridge National Laboratory, TN*

Jun, 2019 **Integrated Computational Materials Education**, *National Science Foundation, UC Berkeley & University of Michigan*

Jul, 2018 **Dislocation Dynamics with Kinetic Monte Carlo**, *Los Alamos National Lab*

Key Skills

Modeling	*Ab initio* (VASP), Finite Element Methods, Kinetic Monte Carlo, Molecular Dynamics
Programming	Java, Python, C++, MATLAB, React, Bash
Machine Learning	Data Analysis, Neural Networks, Feature Engineering
Characterization	Corrosion Analysis, Semiconductor Device Physics

Publications

Huang, S., et al. *Multilayer Interface Tracking Model of Pure Tungsten Oxidation*. **Modelling and Simulation in Materials Science and Engineering** (2022).

Huang, S., et al. *Simulating the Non-Monotonic Strain Response of Nanoporous Multiferroic Composites*. **Applied Physics Letters** (2022).

Nathaniel, J., Huang, S., et al. *Implications of Microstructure in Helium-Implanted Nanocrystalline Metals*. **Materials** (2022).

Huang, S., Karaba, C. T., Patel, et al. *Simulating the non-monotonic strain response of nanoporous multiferroic composites under electric field control*. **Applied Physics Letters** (2022).

Huang, S., Kerrc, R, Murphyc, S, Gilbert, M and Marian, J *Multilayer interface tracking model of pure tungsten oxidation*. **Modelling and Simulation in Materials Science and Engineering** (2022).

Nathaniel, J., El-Atwani, O., Huang, S., Marian, J., *Implications of Microstructure in Helium-Implanted Nanocrystalline Metals*. **Materials** (2022).

Huang, S., and Marian, J. *Rates of diffusion controlled reactions for one-dimensionally-moving species in 3D space*. **Philosophical Magazine** (2019).

Zhao, Y., Zhu, P., Wang, M., Huang, S. et al *A polymerization-assisted grain growth strategy for efficient and stable perovskite solar cells*. **Advanced Materials** (2020).

Jacobs, M., Zhou, X., Olivera, E., Sheil, R., Huang, S., ... and Marian, J. *Room temperature rectification in tapered-channel thermal diodes through nanoscale confinement-induced liquid-solid phase change*. **Journal of Applied Physics** (2021).

Zheng,S, Huang,J, Murali, N., Huang, S., Huang,Y., Jaime Marian, J., et al *New dispersion mechanism for oxide dispersion-strengthened steels by liquid metallurgy*. **Materialia** (2024).

Geng, Peng, Shu Huang, and Jaime Marian., *Stability of trivalent and hexavalent chromium oxide layers on aluminum substrates from electronic structure calculations*. **Physical Review Materials** (2024).