

# Chongze Hu

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## Professional Experience:

- **Assistant Professor (08/2023-Present)**  
Department of Aerospace Engineering and Mechanics, The University of Alabama, Tuscaloosa, AL
- **Postdoctoral Appointee (11/2020-07/2023)**  
Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, NM
- **Adjunct (Part-time) Faculty (01/2022-12/2022)**  
Department of Mechanical Engineering, The University of New Mexico, Albuquerque, NM
- **Summer Visiting Student (06/2017-09/2017 & 06/2014-09/2014)**  
Center of Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, TN

## Education:

- 📖 **University of California San Diego, La Jolla, CA (2017-2020)**  
Ph.D. in Materials Science and Engineering
- 📖 **University of Minnesota-Twin Cities, Minneapolis, MN (2015-2016)**  
M.S. in Mechanical Engineering
- 📖 **Clemson University, Clemson, SC (2012-2015)**  
B.S. in Mechanical Engineering (honor)  
Dual Minors in Physics (honor) and Mathematics

## Research Interests:

- ❖ Computational materials science (e.g., density functional theory, molecular dynamic simulation, and mesoscale phase-field modeling)
- ❖ Computational mechanics, computational nanomechanics, micromechanics
- ❖ Materials informatics, high-throughput modeling, artificial intelligence/machine learning in application to practical problems in materials science and engineering (e.g., advanced manufacturing)
- ❖ Structural ceramics and alloys, high-entropy materials, and energy materials (e.g., thermoelectric materials, semiconductor, battery, etc.)

## Honors and Awards:

- Hewson Engineering Faculty Fellow, The University of Alabama College of Engineering, 2024
- Finalist, 4<sup>th</sup> Rising Star in Computational Materials Science, *Computational Materials Science*, 2022
- Charles A. Dewey, Jr. Endowed Memorial Scholarship, Clemson University, 2014

## Publications: (\*equally contributed, #corresponding author)

Total number of citations: 739; *h*-index: 14; *i*-index:16 (based on Google Scholar as of Feb. 2024)

## Submitted/Under Preparation:

1. **Chongze Hu**, Douglas L. Medlin, Rémi Dingreville. Effect of Segregation on the Stability and Mobility of Grain Boundary Disconnections. ([To be submitted](#))

## Peer-Reviewed Publications:

2. Qizhang Yan, **Chongze Hu**, Jian Luo. Creating Continuously Graded Microstructure via Electrochemically Altering Grain Boundary Complexions. *Materials Today* 2024. DOI: <https://doi.org/10.1016/j.mattod.2024.01.008>.
3. **Chongze Hu**<sup>#</sup>, Rémi Dingreville, Brad L. Boyce. Computational Modeling of Grain Boundary Segregation: A Review. *Comput. Mater. Sci.* 2024, 232, 112596. DOI: <https://doi.org/10.1016/j.commat.2023.112596>.
4. **Chongze Hu**, Stephane Berbenni, Douglas L. Medlin, Rémi Dingreville. Discontinuous Segregation Patterning across Disconnections. *Acta Materialia* 2023, 246, 118724. DOI: <https://doi.org/10.1016/j.actamat.2023.118724>.
5. Yingbin Chen, Luying Huang, **Chongze Hu**, Traian Dumitrica, Hao Xu. Slip Controlled Bending and Rippled Superlattice Design of Few-Layer Graphene. *Applied Surface Science* 2023, 613, 155979. DOI: <https://doi.org/10.1016/j.apsusc.2022.155979>.
6. Fu-Long Li, Zhengming Wu, Yong-Qi Gao, Forrest Z Bowling, J. Matthew Franklin, **Chongze Hu**, Raymond T Suhandynata, Michael A Frohman, Michael V Airola, Huilin Zhou, Kun-Liang Guan. Regulation of PLD1 and PI4KB by ARF GTPases Revealed by Proximal Interaction Network. *The EMBO Journal* 2022, e110698. DOI: <https://doi.org/10.15252/embj.2022110698>.
7. **Chongze Hu**, Shawn Martin, Rémi Dingreville. Accelerating Phase-Field Predictions via Recurrent Neural Networks Learning the Microstructure Evolution in Latent Space. *Comput. Methods Appl. Mech. Eng.* 2022, 397, 115128. DOI: [10.1016/j.cma.2022.115128](https://doi.org/10.1016/j.cma.2022.115128)045-7825.
8. Sashank Shivakumar, Mingde Qin, Dawei Zhang, **Chongze Hu**, Qizhang Yan, Jian Luo. A New Type of Compositionally Complex  $M_5Si_3$  Silicides: Cation Ordering and Unexpected Phase Stability. *Scripta Mater.* 2022, 212, 114557. DOI: <https://doi.org/10.1016/j.scriptamat.2022.114557>.
9. **Chongze Hu**, Jian Luo. Data-Driven Prediction of Grain Boundary Segregation and Disorder in High-Entropy Alloys in a 5-D Space. *Materials Horizons* 2022, 9, 1023-1035. DOI: <https://doi.org/10.1039/D1MH01204E>.
10. Naixie Zhou, **Chongze Hu**, Jian Luo. Grain Boundary Segregation Transitions and Critical Phenomena: A Systematics of Complexion Diagrams with Universal Characters. *Acta Mater.* 2021, 221, 117375. DOI: <https://doi.org/10.1016/j.actamat.2021.117375>.
11. Congying Xiang, Min Shen, **Chongze Hu**, Lok Wing Wong, Hongbo Nie, Huasheng Lei, Jian Luo, Jiong Zhao, Zhiyang Yu. Atomistic Observation of In-Situ Fractured Surface at a V-doped WC-Co Interface. *J. Mater. Sci. Tech.* 2022, 110, 103-108. DOI: <https://doi.org/10.1016/j.jmst.2021.09.021>.
12. **Chongze Hu**, Yanwen Li, Zhiyang Yu, Jian Luo. Computing Grain Boundary Diagrams of Thermodynamics and Mechanical Properties. *npj Comput. Mater.* 2021, 7, 159. DOI: <https://doi.org/10.1038/s41524-021-00625-2>.
13. Min Shen\*, Yanwen Li\*, **Chongze Hu**, Sikang Xue, Congying Xiang, Jian Luo. The Interfacial Structure Underpinning the Al-Ga Liquid Metal Embrittlement: Disorder vs. Order Gradients. *Scripta Mater.* 2021, 204, 114149. DOI: <https://doi.org/10.1016/j.scriptamat.2021.114149>.
14. **Chongze Hu**, Douglas L. Medlin, Rémi Dingreville. Disconnection-mediated Transition in Segregation Structure at Twin Boundaries. *J. Phys. Chem. Lett.* 2021, 12, 6875-6882. DOI: <https://doi.org/10.1021/acs.jpcl.1c02189>.
15. Andrew Wright, Qingyang Wang, **Chongze Hu**, Yi-Ting Yeh, Renkun Chen, Jian Luo. Single-Phase

- Duodenary High-Entropy Fluorite/Pyrochlore Oxides with an Order-Disorder Transition. *Acta Mater.* 2021, 211, 116858. DOI: <https://doi.org/10.1016/j.actamat.2021.116858>.
16. Jiuyuan Nie\*, **Chongze Hu\*** (equally contributed), Qizhang Yan, Jian Luo. Discovery of Electrochemically Induced Grain Boundary Transitions. *Nature Commun.* 2021, 12, 2374. DOI: <https://doi.org/10.1038/s41467-021-22669-0>.  
**Editors' highlights:** <https://www.nature.com/collections/eecgdgijhh>.
  17. Can Yang\*, **Chongze Hu\*** (equally contributed), Xinfu Gu, Hongbo Ni, Congyin Xiang, Lin Xie, Jiaqing He, Wenqing Zhang, Zhiyang Yu, Jian Luo. Interfacial Superstructures and Chemical Bonding Transitions at Metal-Ceramics Interfaces. *Science Advances* 2021, 7, 11. DOI: [10.1126/sciadv.abf6667](https://doi.org/10.1126/sciadv.abf6667).
  18. **Chongze Hu**, Andrei Dernov, Hao Xu, Grigorii Drozdov, Traian Dumitrica. *Ab Initio* Predictions of a Graphite-like Phase of Collapsed Carbon Nanotubes with Anomalous Grain Boundaries and Flexoelectricity. *J. Chem. Phys.* 2021, 154, 044701. DOI: <https://doi.org/10.1063/5.0038666>.
  19. Yanwen Li, Hongbo Nie, Sikang Xue, **Chongze Hu**, Congying Xiang, Xiaohui Su, Jian Luo, Zhiyang Yu, Siwei Li. Abnormal Grain Growth in Iron-Containing SiC Fibers. *J. Europ. Ceram. Soc.* 2021, 41, 2306-2311. DOI: <https://doi.org/10.1016/j.jeurceramsoc.2020.12.007>.
  20. Congying Xiang, Chao Liu, Xiao Wen, Hongbo Nie, **Chongze Hu**, Zhishan Luo, Yanwen Li, Jian Luo, Zhiyang Yu. Formation of Stacking Faults in Tungsten Carbide during Sintering. *Ceram. Int.* 2020, 46, 15851-15857. DOI: <https://doi.org/10.1016/j.ceramint.2020.03.132>.
  21. Mingde Qin, Qizhang Yan, Haoren Wang, **Chongze Hu**, Kenneth Vecchio, Jian Luo. High-Entropy Monoborides: Towards Superhard Materials. *Scripta Mater.* 2020, 189, 101-105. DOI: <https://doi.org/10.1016/j.scriptamat.2020.08.018>.
  22. Mingde Qin, Joshua Gild, **Chongze Hu**, Haoren Wang, Md Shafkat Bin Hoque, Jeffrey Braun, Tyler Harrington, Patrick Hopkins, Kenneth Vecchio, Jian Luo. Dual-Phase High-Entropy Ultrahigh Temperature Ceramics. *J. Europ. Ceram. Soc.* 2020, 40, 5037-5050. DOI: <https://doi.org/10.1016/j.jeurceramsoc.2020.05.040>.
  23. **Chongze Hu**, Yunxing Zuo, Chi Chen, Shyue Ping Ong, Jian Luo. Genetic Algorithm-Guided Deep Learning of Grain Boundary Diagrams: Addressing the Challenge of Five Degrees of Freedom. *Materials Today* 2020, 38, 49-57. DOI: <https://doi.org/10.1016/j.mattod.2020.03.004>.
  24. Zhishan Luo\*, **Chongze Hu\*** (equally contributed), Lin Xie, Hongbo Nie, Congying Xiang, Xinfu Gu, Jiaqing He, Wenqing Zhang, Zhiyang Yu, Jian Luo. A Highly Asymmetric Interfacial Superstructure in WC: Expanding the Classic Grain Boundary Segregation and New Complexion Theories. *Materials Horizons* 2020, 7, 173-180. DOI: <https://doi.org/10.1039/C9MH00969H>.
  25. **Chongze Hu**, Jian Luo. First-Order Interfacial Transition in Si-Au Binary System: Hybrid Monte Carlo and Molecular Dynamics Simulations Verified by First-Principles Calculations. *Scripta Mater.* 2019, 158, 11-15. DOI: <https://doi.org/10.1016/j.scriptamat.2018.08.017>.
  26. Xiangguo Li, **Chongze Hu**, Chi Chen, Zhi Deng, Jian Luo, Shyue Ping Ong. Quantum-Accurate Spectral Neighbor Analysis Potential Models for Ni-Mo Binary Alloys and FCC Metals. *Phys. Rev. B* 2018, 98, 094104. DOI: <https://doi.org/10.1103/PhysRevB.98.094104>.
  27. **Chongze Hu**, Jingsong Huang, Bobby G. Sumpter, Efsthathios Meletis, Traian Dumitrica. *Ab Initio* Predictions of Strong Interfaces in Transition-Metal Carbides and Nitrides for Superhard Nanocomposite Coating Applications. *ACS Appl. Nano Mater.* 2018, 5, 2029-3025. DOI: [10.1021/acsanm.8b00227](https://doi.org/10.1021/acsanm.8b00227).

28. **Chongze Hu**, Peter Ni, Li Zhan, Huijuan Zhao, Jian He, Jingsong Huang, Bobby G. Sumpter. Theoretical Investigation of Electrical Transport Properties in CoSb<sub>3</sub> Skutterudites under Hydrostatic Loadings. *Rare Metal* 2018, 37, 316-325. DOI: <https://doi.org/10.1007/s12598-018-1000-7>.
29. **Chongze Hu**, Jingsong Huang, Bobby G. Sumpter, Efstathios Meletis, Traian Dumitrica. Ab Initio Predictions of Hexagonal Zr(B,C,N) Polymorphs for Coherent Interface Design. *J. Phys. Chem. C* 2017, 121, 26007-26018. DOI: [10.1021/acs.jpcc.7b09444](https://doi.org/10.1021/acs.jpcc.7b09444).
30. **Chongze Hu**, Xiaoyu Zeng, Yufei Liu, Menghan Zhou, Huijuan Zhao, Terry M. Tritt, Jian He, Jacek Jakowski, J.; Paul R. C. Kent, Jingsong Huang, Bobby G. Sumpter. Effects of Partial La Filling and Sb Vacancy Defects on CoSb<sub>3</sub> Skutterudites. *Phys. Rev. B* 2017, 95, 165204. DOI: <https://doi.org/10.1103/PhysRevB.95.165204>.
31. Ying Liu, **Chongze Hu**, Jingsong Huang, Bobby G. Sumpter, and Rui Qiao. Tuning Interfacial Thermal Conductance of Graphene Embedded in Soft Materials by Vacancy Defects. *J. Chem. Phys.* 2015, 142, 244703. DOI: <http://dx.doi.org/10.1063/1.4922775>.

### **Invited Talks/Presentations:**

1. “Interfacial Superstructure of Segregation in Tungsten Carbide”, ICACC, Daytona Beach, Feb. 2024.
2. “Accelerating Phase-Field Prediction via Recurrent Neural Networks for Microstructural Evolution”, Applied Math Seminar, The University of Alabama, Nov. 2023.
3. “Discontinuous Segregation Patterning Across Disconnections”, CINT Seminar, Sandia National Laboratories, Jun. 2023.
4. “Accelerating Multiscale Materials Modeling via Machine Learning: From Computing Grain Boundary Diagrams to Microstructure Prediction”, College of Engineering, University of North Carolina at Charlotte, Mar. 2023.
5. “Accelerating Multiscale Materials Modeling via Machine Learning: From Computing Grain Boundary Diagrams to Microstructure Prediction”, Department of Mechanical Engineering, University of Texas Rio Grande Valley, Feb. 2023.
6. “Multiscale Materials Modeling and Machine Learning for Grain Boundaries (GBs)”, Department of Mechanical Engineering, Texas Tech University, Nov. 2022.
7. “Modeling General Grain Boundaries (GBs): From Computing GB Diagrams via Atomistic Simulation to Machine Learning to GB Transition”, Graduate Seminar, Department of Mechanical Engineering, University of New Mexico, Oct. 2021.
8. “Modeling General Grain Boundaries (GBs): From Computing GB Diagrams via Atomistic Simulation to Machine Learning to GB Transition”, Department of Mechanical Engineering, Louisiana State University, Mar. 2021.
9. “Modeling General Grain Boundaries (GBs): From Computing GB Diagrams to Understanding GB Superstructures and an Electric Field Induced GB Transition”, ICACC, Daytona Beach, Jan. 2020.

### **Other Conference Talks/Poster Presentations:**

1. “Discontinuous Segregation Patterning Across Disconnections: A Combined Atomistic Simulation and Continuum Modeling Study”, TMS, San Diego, 2023. (Oral)
2. “Disconnection-Mediated Transition in Segregation Structure at Twin Boundaries: A Molecular Dynamic Simulation of Platinum-Gold System”, TMS, Anaheim, 2022. (Oral)
3. “Computing Grain Boundary Diagrams for High-Entropy Alloys”, TMS, Anaheim, 2022. (Oral)
4. “Disconnection-Mediated Transition in Segregation Structure at Twin Boundaries: A Molecular Dynamic Simulation of Platinum-Gold System”, CINT 2021 User Meeting, Sandia National Laboratories, 2021.

(Poster)

5. “Computing Grain Boundary Diagrams”, TMS, San Diego, 2020. (Oral)
6. “Computing Grain Boundary Diagrams”, Golden Research Conference, South Hadley, 2018. (Poster)
7. “Development of Interfacial “Phase” Diagrams for the Materials Genome Initiative: Tailing the Processing and Properties of Materials for Defense Applications”, Vannevar Bush Faculty Fellowship 10<sup>th</sup> Anniversary Program Review, DC, 2018. (Poster)
8. “Stress Effect on Electronic and Thermoelectric Properties of Skutterudite”, Joint Nanoscience and Neutron Scattering User Meeting, ORNL, 2017. (Poster)
9. “Ab Initio Explorations of a New Class of Quaternary ZrBCN Nanocomposite Coatings for Harsh Environments”, Joint Nanoscience and Neutron Scattering User Meeting, ORNL, 2017. (Poster)
10. “Experimental and Theoretical Studies of La Filled CoSb<sub>3</sub> Kieftite”, APS/CNMS User Meeting, ORNL, 2016. (Poster)
11. “Probing the Role of La Fillers and Sb Vacancies in CoSb<sub>3</sub> Skutterudites”, International Conference of Thermoelectric, Wuhan, August 2016. (Oral)

### **Professional Membership:**

- American Ceramics Society (ACerS)
- The Minerals, Metals & Materials Society (TMS)
- American Physical Society (APS)

### **Service/Professional/Synergistic Activities:**

- Committee member for Ph.D. dissertation defense, Department of Aerospace Eng. and Mechanics, UA
- Committee member for Ph.D. qualify exam, Department of Aerospace Eng. and Mechanics, UA
- Committee member of 2024 International Conference on Aerospace and Mechanics (ICAM 2024).
- Panel reviewer: NSF reviewer 2024, DOE reviewer 2024.
- Young editorial board member for *Rare Metal* (IF: 8.8), 2022-Present
- Guest editor for *Metals* Special Issue on “Mechanical Behaviors and Interfacial Segregation Phenomena in Metallic Materials: Simulation, Theory, and Characterization”, 2024.
- Journal Reviewer for *Journal of Nuclear Materials*, *Computational Materials Science*, *Journal of Materials Science & Technology*, *Rare Metal*, *Mechanics of Materials*, *Physical Review Materials*, *Physical Review B*, and *Results in Materials*.

### **Teaching/Mentoring Experience:**

- Instructor for *AEM453/553 Multiscale Analysis for Advanced Composites*, Department of Aerospace Engineering and Mechanics, The University of Alabama, Spring 2024.
- Instructor for *AEM530 Continuum Mechanics*, Department of Aerospace Engineering and Mechanics, The University of Alabama, Fall 2023.
- Instructor for *ME471&571 Advanced Materials Science*, Department of Mechanical Engineering, University of New Mexico, Fall 2022. Course evaluation: 5.0/5.0.
- Instructor for *ME459 Mechanical Engineering Design IV*, Department of Mechanical Engineering, University of New Mexico, Spring 2022. Course evaluation: 3.5/5.0.
- Graduate Teaching Assistant for *Computational Nano-Mechanics Course*, Department of Mechanical Engineering, University of Minnesota-Twin Cities, Spring 2016.

### **Community Outreach:**

- Teaching Assistant for *HMTech* 2021 Summer STEM Program for African American Middle and High School Students, Summer 2021.