Zhenze Yang

Sept. 2022
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EDUCATION

Massachusetts Institute of Technology (MIT), Cambridge, USA 2019/09- present
Doctor of Philosophy, Department of Materials Science and Engineering
GPA: 4.8/5.0
Advisor: Markus J. Buehler

University of Chinese Academy of Science (UCAS), China 2015/09- 2019/07
Bachelor of Science, Department of Physics
GPA: 3.96/4.0; **ranking:** 1/92

RESEARCH EXPERIENCES

Graduate Research Assistant, DMSE, MIT 2019/09 - present
Advisor: **Markus J. Buehler**

- **Overview**: Combined machine learning with multiscale simulations for accelerated property calculations and designs of diverse materials including composite materials (two-phase composites), nanomaterials (graphene, MXene) and biological materials (proteins, spider silk).
- **Project 1**: Developed a cGAN-based approach for direct translation from composite microstructures to strain/stress fields, serving as alternatives to FEA. (Z. Yang et al. ***Sci. Adv***. 2021; Z. Yang et al. ***JMPS***. 2021)
- **Project 2**: Developed a GNN-based method for linking structural defects to atomic properties for crystalline solids, showing advantages over MD simulations. (Z. Yang et al. ***Npj Comput. Mater***. 2022)
- **Project 3**: High-throughput generation of graphene foams and property quantification based on machine learning. (Z. Yang et al. ***Small Methods***. 2022)
- **Project 4**: Generative designs of diverse materials from architected materials to protein-based materials (Z. Yang et al. ***Front. Mater***. 2021. Z. Yang et al. ***APL. Mater***. 2022. Z. Yang et al. ***JMPS (in review)***. 2022)

Undergraduate Thesis Defense, UCAS 2019/02 – 2019/07
Supervisor: **Jure Dobnikar**

- **Overview**: Utilized coarse-grained models for selective transport of biomolecules through nuclear pore complex. Revealed the relation between transport likelihood with diverse factors such as particle size, polymer density and interactions.

Undergraduate Research Assistant, UC Berkeley 2018/09 – 2019/02
Supervisor: **Mohammad R.K. Mofrad**

- **Overview**: Utilized molecular dynamics simulation for dynamic chromatin folding. Revealed the minimal size and loop length variation with respect to the folding dynamics. Reproduced the experimental observations from Hi-C technology. (Z Yang et al. ***bioRxiv***. 2020)

Undergraduate Research Assistant, MIT 2018/06 – 2018/08
Supervisor: **Alfredo Alexander-Katz**

- **Overview**: Developed automatic program to accomplish 3D reverse engineering of a block copolymer system combing the coarse-grained modeling. Implemented particle swarm algorithm for optimizing the parameters which affect the phase of block copolymer assemblies.

Undergraduate Research Assistant, Institute of Physics, CAS 2017/09 – 2018/05
Supervisor: **Sheng Meng**

- **Overview**: Experiments on wetting behavior of water droplets on thermoelectric surface. Revealed the nominal variations of contact angles of water droplets on charged surface (Y. Shen et al. ***Chin. Phys. B***. 2022).

Research Assistant, Technical Institute of Physics and Chemistry, CAS 2017/07 – 2017/10

Supervisor: **Jing Liu**

- **Overview**: Experiments on biomimetic crawling of liquid metal droplets. Revealed the mechanism of spreading-wetting behaviors by formation of intermetallic surfaces. (Y. Cui et al. ***ACS Appl. Mater. Interfaces***. 2022)

PUBLICATIONS

- **Z. Yang**, YC. Hsu**,** M. J. Buehler, "Generative multiscale analysis of de novo proteome-inspired molecular structures and nanomechanical optimization using a VoxelPerceiver transformer model", ***JMPS. In review***, 2022.
- B. Ni, D. Steinbach, **Z. Yang**, A. Lew, B. Zhang, Q. Fang, M. J. Buehler, J. Lou, "Fracture at the Two-Dimensional Limit", ***MRS Bull. In press***, 2022.
- **Z. Yang**, M. J. Buehler, "Linking Atomic Structural Defects to Mesoscale Properties in Crystalline Solids using Graph Neural Networks", ***Npj Comput. Mater.***, 2022, 8(198).
- CH. Yu, BY. Tseng, **Z. Yang**, CC. Tung, E. Zhao, ZF. Ren, SS. Yu, PY. Chen, CS. Chen, M. J. Buehler. "Hierarchical Multiresolution Design of Bioinspired Structural Composites Using Progressive Reinforcement Learning", ***Adv. Theory Simul.***, 2022: 2200459.
- W. Lu, **Z. Yang**, M. J. Buehler, "Rapid Mechanical Property Prediction and de novo Design of Three-dimensional Spider Webs Though Graph and GraphPerceiver Neural Networks", ***JAP***, 2022, 132(7), 074703. (Featured by Scilight)
- **Z. Yang**, M. J. Buehler, "High-throughput Generation of Three-dimensional Graphene Metamaterials and Property Quantification Using Machine Learning", ***Small Methods***, 2022: 2200537.
- Y. Sheng, T. Lin, **Z. Yang**, Y. Huang, J. Xu, S. Meng, "Water Contact Angles on Charged Surfaces in Aerosols". ***Chin. Phys. B***, 2022, 31(5): 056801.
- YC. Hsu*, **Z. Yang***, M. J. Buehler, "Generative Design, Manufacturing, and Molecular Modeling of 3D Architected Materials Based on Natural Language Input". ***APL Mater.***, 2022, 10(4): 041107.
- S. Gong, S. Wang, T. Zhu, X. Chen, **Z. Yang**, M. J. Buehler, Y. Shao-Horn, J. C. Grossman. "Screening and Understanding Li Adsorption on Two-Dimensional Metallic Materials by Learning Physics and Physics-Simplified Learning". ***JACS Au***, 2021, 1(11): 1904-1914.
- **Z. Yang**, M. J. Buehler, "Words to Matter: De novo Architected Materials Design Using Transformer Neural Networks". ***Front. Mater.***, 2021, 8: 740754. (Featured by MIT CEE News)
- **Z. Yang**, CH. Yu, Kai Guo, Markus J. Buehler, "End to End Deep Learning Method to Predict Complete Strain and Stress Tensors for Complex Hierarchical Composite Microstructures", ***JMPS***, 2021, 154: 104506.
- **Z. Yang***, CH. Yu*, M. J. Buehler**, "**Deep Learning Model to Predict Complex Stress and Strain Fields in Hierarchical Composites", ***Sci. Adv.***, 2021, 7(15): eabd7416. (Featured by MIT News, EurekAlert!, Phys.org, ScienceDaily and SciTechDaily)
- K. Guo, **Z. Yang**, M. J. Buehler, "Artificial Intelligence and Machine Learning in Mechanical Design of Materials", ***Mater. Horiz.***, 2021, 8(4): 1153-1172.
- Y. Cui†, F. Liang‡, **Z. Yang**, S. Xu, X. Zhao, Y. Ding, Z. Lin, J. Liu, "Metallic Bond Enabled Wetting Behavior at the Liquid Ga/CuGa2 Interfaces", ***ACS Appl. Mater. Interfaces***, 2018, 10 (11): 9203-9210
- Y. Cui, Y. Ding, S. Xu, **Z. Yang**, P. Zhang, W. Rao, J. Liu, "Liquid Metal Corrosion Effects on Conventional Metallic Alloys Exposed to Eutectic Gallium–Indium Alloy Under Various Temperature States", ***Int. J. Thermophys.***, 2018, 39(10): 1-14.

HONORS AND AWARDS

Outstanding graduate award of Beijing	2019/07
Tang Lixin Scholarship	2018/07
First class scholarship (Top 5%) of 2017-2018 Academic Year	2018/10
First class scholarship (Top 5%) of 2016-2017 Academic Year	2017/10
First class scholarship (Top 5%) of 2015-2016 Academic Year	2016/10

SKILLS

- Proficient in machine learning, deep learning approaches (CNN, RNN, GANs, GNN, Transformer, etc.) and optimization methods (genetic algorithms, particle swarm algorithm).
- Proficient in Molecular Dynamics Simulation, Finite Element Analysis, Density Functional Theory.
- Proficient in Python and C programming, frequent user of LAMMPS, ABAQUS, Matlab, Quantum Espresso.