Zhenze Yang

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Laboratory of Atomistic and Molecular Mechanics, MIT, Cambridge, MA-02139
Tel: (+1) 617-710-8895 Email: zhenzey@mit.edu

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 California, Berkeley, Berkeley 2018/08 – 2019/02
Exchange program, Department of Physics

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

WORKING EXPERIENCES

Summer Intern, Toyota Research Institute, Los Altos, CA 2023/06 – 2023/08
Team: High-throughput polymer team, Energy & Materials Division.

- **Overview**: Applied generative AI models to generate polymer electrolytes with high ionic conductivity.

RESEARCH EXPERIENCES

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

- **Overview**: Combined **machine learning** with **multiscale simulations** (MD, FEM) for accelerated property calculations and designs of diverse materials including composite materials (two-phase composites), nanomaterials (graphene-based materials, MXene) and biological materials (proteins, polypeptides).

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.

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.

Undergraduate 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.

PUBLICATIONS

1. **Zhenze Yang**, Sarah Yorke, Markus J. Buehler, Tuomas Knowles. "Multi-fidelity machine learning for solving polypeptide sequence challenge", ***In preparation.***
2. **Zhenze Yang**, Weike Ye, Xiangyun Lei, Daniel Schweigert, Ha-Kyung Kwon, Arash Khajeh. "*De novo* design of polymer electrolyte with high ionic conductivity using GPT-based and diffusion-based generative models", ***Submitted.***
3. **Zhenze Yang***, Sarah Yorke*, Elizabeth Wiita*, Markus J. Buehler, Tuomas Knowles, "Sustainable Polypeptide Material Systems", ***Nature Review Materials, In review***, 2023
4. **Zhenze Yang**, Markus J. Buehler, "Fill in the Blank: Transferrable Deep Learning Approaches to Recover Missing Physical Field Information", ***Advanced Materials***, 2023: 2301449. (Featured by MIT News).
5. **Zhenze Yang**, Yu-Chuan Hsu**,** Markus J. Buehler, "Generative multiscale analysis of de novo proteome-inspired molecular structures and nanomechanical optimization using a VoxelPerceiver transformer model", ***Journal of the Mechanics and Physics of Solids,*** 2023, 170: 105098.
6. **Zhenze Yang**, Markus J. Buehler, "High-throughput Generation of Three-dimensional Graphene Metamaterials and Property Quantification Using Machine Learning", ***Small Methods***, 2022: 2200537.
7. **Zhenze Yang**, Markus J. Buehler, "Linking Atomic Structural Defects to Mesoscale Properties in Crystalline Solids using Graph Neural Networks", ***Npj Computational Materials.*** 2022, 8(198).
8. **Zhenze Yang*****,** Yu-Chuan Hsu***,** Markus J. Buehler, "Generative Design, Manufacturing, and Molecular Modeling of 3D Architected Materials Based on Natural Language Input". ***APL Materials***, 2022, 10(4): 041107.
9. **Zhenze Yang**, Markus J. Buehler, "Words to Matter: De novo Architected Materials Design Using Transformer Neural Networks". ***Frontiers in Materials***, 2021, 8: 740754. (Featured by MIT CEE News)
10. **Zhenze Yang**, Chi-Hua Yu, Kai Guo, Markus J. Buehler, "End to End Deep Learning Method to Predict Complete Strain and Stress Tensors for Complex Hierarchical Composite Microstructures", ***Journal of the Mechanics and Physics of Solids***, 2021, 154: 104506.
11. **Zhenze Yang***, Chi-Hua Yu*, Markus J. Buehler**, "**Deep Learning Model to Predict Complex Stress and Strain Fields in Hierarchical Composites", ***Science Advances***, 2021, 7(15): eabd7416. (Featured by MIT News, EurekAlert!, Phys.org, ScienceDaily and SciTechDaily)
12. **Zhenze Yang,** Mohammad R.K. Mofrad, "The intriguing dynamics of chromatin folding and assembly", ***bioRxiv***, 2020.
13. Bo Ni, Doug Steinbach, **Zhenze Yang**, Andrew Lew, Boyu Zhang, Qiyi Fang, Markus J. Buehler, Jun Lou, "Fracture at the Two-Dimensional Limit", ***MRS Bulletin***, 2022, 47(8): 848-862.
14. Chi-Hua Yu, Bor-Yann Tseng, Zhenze Yang, Cheng-Che Tung, Elena Zhao, Zhi-Fan Ren, Sheng-Sheng Yu, Po-Yu Chen, Chuin-Shan Chen, and Markus J. Buehler. "Hierarchical Multiresolution Design of Bioinspired Structural Composites Using Progressive Reinforcement Learning", ***Advanced Theory and Simulations***, 2022: 2200459.
15. Wei Lu, **Zhenze Yang**, Markus J. Buehler, "Rapid Mechanical Property Prediction and de novo Design of Three-dimensional Spider Webs Though Graph and GraphPerceiver Neural Networks", ***Journal of Applied Physics***, 2022, 132(7), 074703. (Featured by Scilight)
16. Yutian Sheng, Ting Lin, **Zhenze Yang**, Yongfeng Huang, Jiyu Xu, Sheng Meng, "Water Contact Angles on Charged Surfaces in Aerosols". ***Chinese Physics B***, 2022, 31(5): 056801.

17. Sheng Gong, Shuo Wang, Taishan Zhu, Xi Chen, **Zhenze Yang**, Markus J. Buehler, Yang Shao-Horn, Jeffrey 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.
18. Kai Guo, **Zhenze Yang**, Markus J. Buehler, "Artificial Intelligence and Machine Learning in Mechanical Design of Materials", ***Materials. Horizons***, 2021, 8(4): 1153-1172.
19. Yuntao Cui†, Fei Liang‡, **Zhenze Yang**, Shuo Xu, Xi Zhao, Yujie Ding, Zheshuai Lin, Jing Liu, "Metallic Bond Enabled Wetting Behavior at the Liquid Ga/CuGa2 Interfaces", ***ACS applied materials & interfaces***, 2018, 10 (11): 9203-9210
20. Yuntao Cui, Yujie Ding, Shuo Xu, **Zhenze Yang**, Pengju Zhang, Wei Rao, Jing Liu, "Liquid Metal Corrosion Effects on Conventional Metallic Alloys Exposed to Eutectic Gallium–Indium Alloy Under Various Temperature States", ***International Journal of Thermophysics***, 2018, 39(10): 1-14.

TEACHING & MENTORING

Teaching Assistant, MECHE/CEE, MIT 2023/03 – 2023/05

- TAing new Undergraduate/graduate-level course "Advancing Mechanics and Materials via Machine Learning" (Instructor: Prof. Markus J. Buehler).

Research Mentor, Undergraduate Research Opportunities Program (UROP), MIT 2021/02 – 2021/05

- Mentoring MIT senior undergraduate Antony Hernandez (EECS, MIT) on research topic "Deep Learning Model to Predict Strain/stress field in 3D Hierarchical Composites".

Academic Mentor, MIT 2019/09 – present

- Mentoring undergraduate students from different universities and providing consulting for their PhD applications.
- Mentored students
  - Yuetan Chu (University of Science and Technology of China);
  - Yuheng Xie (University of Science and Technology of China);
  - Danyi Zhang (University of Chinese Academy of Sciences);
  - Simeng Yu (Peking University);
  - Zan Yin (Tsinghua University);
  - Xinzhe Dai (University of Chinese Academy of Sciences).

SELECTED PRESENTATION

- "Deep Learning Model to Predict Complex Stress and Strain Fields in Hierarchical Composites", ***USNCCM16***, June 2021 (Virtual).
- "Deep Learning Model to Predict Complex Stress and Strain Fields in Hierarchical Composites", ***MRS Fall 2021***, Dec 2021 (Virtual).
- "High-throughput Generation of 3D Graphene Metamaterials and Property Quantification Using Machine Learning", ***SES2022***, Oct 2022 (College station, TX).
- "Fill in the Blank: Transferrable Deep Learning Approaches to Recover Missing Physical Field Information", ***SES2023***, Oct 2023 (Minneapolis, Mn).
- "*De novo* design of polymer electrolyte with high ionic conductivity using GPT-based and diffusion-based generative models", ***MRS2023***, Nov 2023 (Boston, MA).

ACADEMIC SERVICE

Reviewer for Scientific Journals (reviewed 15+ articles): Proceedings of the National Academy of Sciences; Journal of Mechanical Behaviors of Biomedical Materials; APL Machine Learning; Journal of Cheminformatics; Mechanics of Materials; Frontier in Bioengineering and Biotechnology; AIP Advances; Computational Materials Science; PLOS One; Materials Science Forum.

RESEARCH SUMMARY

AI-based Surrogate Model for Mechanical Materials

- **"Structure-physical field" linkage:** While massive "AI-for-science" studies focus on learning "structure-property" relation, my PhD research focus on developing DL-based methods for so-called "structure-physical field" linkage. The physical field can be strain/stress fields, potential energy or electron density distributions. The reasons I am interested in physical field prediction are: 1) Physical field contains more comprehensive information compared to a single material property; 2) Derivative properties can be calculated from physical field (e.g. from stress field to Young's modulus).
- **AI-based surrogate model bypassing FEA calculation:** I proposed a conditional generative adversarial network (cGAN)-based approach to realize end-to-end translation from composite geometry to strain/stress fields without any requirement of domain knowledge. I showed that the model bypasses FEA with better efficiency and possesses great generality regardless of component microstructures, boundary conditions and geometric hierarchy. I further validated the approach with well-established linear elasticity theory. Besides forward problem, I also developed a framework that tackle with challenging inverse problems, enabling geometry identification from incomplete mechanical behaviors and proposed a potential solution for ill-posed situation.
- **AI-based surrogate model bypassing MD simulation:** I built a graph neural network-based model that can learn the "structure-physical field" linkage in crystalline solids at atomic scale, serving as an accelerated alternative to molecular dynamics simulations. I tested the model on different types of structural defects such as dislocation and vacancy and different nanocrystals including 2D graphene and 3D aluminum, indicating the robustness of the method. In addition, I combined the surrogate model with certain evolutionary optimization algorithm, enabling design of nanoporous graphene membrane.

High-throughput Virtual Generation

- **Tailoring nanomaterials:** Using high-throughput atomistic MD simulations, I curated multiple computational datasets for graphene-based materials including polycrystalline and porous 2D graphene flakes and 3D graphene foams. With these datasets, I was able to study their mechanical behaviors and relate structural defects to their performances. Furthermore, I leveraged both classical ML algorithms and DL methods to predict their properties from structures. The datasets I created and the AI-based predictive tools can be utilized to study graphene-based materials and provide guidance to experimental synthesis and design.
- **Formulating biological materials:** Using coarse-grained MD simulations, I calculated the Young's modulus of polypeptide self-assemblies with different amino acid sequences and built a dataset on top of it. I also collected properties of polypeptide systems from existing studies by literature mining. With the data, I performed multi-fidelity machine learning, leveraging both high-fidelity, small amount of experimental data and low-fidelity, large amount of computational data to build the model for solving "polypeptide sequence challenge".

Generative Design of Functional Materials

- **Pretrained foundation model for metamaterials design:** With the boom of large language and vision models, there are massive generative toolboxes that can create new text documents and fancy images. I utilized these large pretrained models to design architected materials. By simply giving these models text prompts or bio-inspired ideas, I revealed that these models, although not developed specifically for materials science, can generate unseen metamaterials beyond intuition. Furthermore, I examined these proposed design candidates with multiscale simulations and additive manufacturing, showing interesting deformation mechanism in these functional materials.
- **Generative AI for designing battery materials:** I also applied my domain knowledge and expertise in industrial context by applying generative AI to design polymer electrolytes during an intern at Toyota. I proposed a conditional generation framework that enables searching for polymer electrolytes with desirable properties like high ionic conductivity. I compared different DL architectures from GPT to diffusion models and also performed a pretraining & fine-tuning strategy which largely enhances the performance of generative AIs in creating new polymers. The proposed promising polymers have the potential to become next-generation battery materials.