

# BO NI

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## EDUCATION

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|--------------------------------------------------------------------------|-------------------|
| <b>Brown University</b> , Providence, RI                                 | 09/2013 – 05/2021 |
| Ph.D. in Mechanical Engineering                                          |                   |
| Dissertation: <i>Topological toughening and fracture of 2D materials</i> |                   |
| Advisor: Prof. Huajian Gao [ <a href="#">website</a> ]                   |                   |
| <b>Xi'an Jiaotong University (XJTU)</b> , Xi'an, Shaanxi province, China | 09/2011 – 07/2013 |
| M.Sc. in Solid Mechanics                                                 |                   |
| <b>Xi'an Jiaotong University (XJTU)</b> , Xi'an, Shaanxi province, China | 09/2007 – 05/2011 |
| B.Sc. in Engineering Mechanics                                           |                   |

## RESEARCH INTERESTS

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Multiscale modeling, generative artificial intelligence (GenAI), protein design and mechanics, alloy design for additive manufacturing (AM), fracture and friction in two-dimensional (2D) materials, topological defect and toughening

## RESEARCH EXPERIENCE

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| <b>Postdoctoral researcher</b> , <i>Carnegie Mellon University (CMU)</i>                                                                                                                                                                                                                                                                 | 01/2024 – present |
| Principal Investigator: Prof. Mohadeseh Taheri-Mousavi [ <a href="#">website</a> ]                                                                                                                                                                                                                                                       |                   |
| Project: <b>generative AI for additive manufacturable alloy design in extreme environments</b>                                                                                                                                                                                                                                           |                   |
| <ul style="list-style-type: none"><li>• Generalize large language models (LLMs) for alloy composition design</li><li>• Automate alloy discovery and processing via LLM-powered <i>multi-agent</i> collaborations</li></ul>                                                                                                               |                   |
| <b>Postdoctoral researcher</b> , <i>Massachusetts Institute of Technology (MIT)</i>                                                                                                                                                                                                                                                      | 07/2021 – 12/2023 |
| Principal Investigator: Prof. Markus Buehler [ <a href="#">website</a> ]                                                                                                                                                                                                                                                                 |                   |
| Project I: <b><i>de novo</i> protein design using GAI</b>                                                                                                                                                                                                                                                                                |                   |
| <ul style="list-style-type: none"><li>• Build protein structural and mechanical databases via parallel full-atom simulations</li><li>• Develop end-to-end protein predictors and designers using language diffusion models</li><li>• Inverse design <i>de novo</i> proteins that meet desired structural/mechanical properties</li></ul> |                   |
| Project II: <b>merging deep learning (DL) and physics-based modeling</b>                                                                                                                                                                                                                                                                 |                   |
| <ul style="list-style-type: none"><li>• Detect internal cracks based on deformation on the boundaries using DL models</li><li>• Solve elasticity problems automatically via LLM multi-agent conversations</li></ul>                                                                                                                      |                   |

Advisor: Prof. Huajian Gao [[website](#)]

**Project I: fracture and toughening of 2D materials**

- Explain toughening mechanisms in rebar graphene experiments using modeling
- Analyze crack and asymmetric edge stress interaction in h-BN using analytical theories
- Model nonlinear couplings between topological defects, curvature and crack in graphene via molecular dynamics and phase field simulations

**Project II: shell-based multi-stable nanolattice design**

- Implement snap-through instability & multi-stable states in 3D graphene via modeling
- Develop theories for rational design of pseudo plasticity in brittle 3D graphene

**Project III: fracture in lithium-ion batteries**

- Explain counterintuitive crack-inclusion interactions under an applied T-stress using Eshelby mechanics theories.

**Project IV: solving inverse problems in mechanics using DL approaches**

- Generalize conditional generative adversarial net (c-GAN) model to solve elastic modulus identification problem for non-destructive evaluation

**JOURNAL PUBLICATIONS** [[Google Scholar link](#)]

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**Under review and preprints**

1. [Ni, B.](#) and Buehler, M.J., 2025. Agentic End-to-End De Novo Protein Design for Tailored Dynamics Using a Language Diffusion Model, arXiv preprint arXiv:2502.10173, under review. [[code](#)]
2. [Ni, B.](#), and Taheri-Mousavi, S. M., 2025. Accelerate materials discovery and design via generative artificial intelligence, under review.

**Research articles**

3. [Ni, B.](#), Glaser, B., Taheri-Mousavi, S. M., 2025. End-to-end prediction and design of additively manufacturable alloys using a generative AlloyGPT model, *npj Computational Materials*, 11(1), 294. [[code](#)] (Highlighted by CMU News [[website](#)])
4. Shin, B.\*, [Ni, B.](#)\*, Toh C.\*, Steinbach, D., Yang, Z., Sassi, L., Ai, Q., Niu, K., Lin, J., Suenaga, K., Han, Y., Buehler, M.J., Özyilmaz, B. and Lou, J., 2025. Intrinsic toughening in monolayer amorphous carbon nanocomposites, *Matter*. (\*Co-first authors) (Highlighted by Rice News [[website](#)])
5. [Ni, B.](#) and Buehler, M.J., 2024. MechAgents: Large language model multi-agent collaborations can solve mechanics problems, generate new data, and integrate knowledge. *Extreme Mechanics Letters*, 67, p.102131. [[code](#)]
6. [Ni, B.](#), Kaplan, D.L. and Buehler, M.J., 2024. ForceGen: End-to-end de novo protein generation based on nonlinear mechanical unfolding responses using a protein language diffusion model. *Science Advances* 10(6): eadl4000. [[code](#)]
7. [Ni, B.](#), Kaplan, D.L. and Buehler, M.J., 2023. Generative design of de novo proteins based on

secondary-structure constraints using an attention-based diffusion model. *Chem*, 9(7), pp.1828–1849. (Selected as the [issue cover](#)) (Highlighted by MIT news [\[website\]](#)) [\[code\]](#)

8. Liu, F.Y., [Ni, B.](#) and Buehler, M.J., 2022. PRESTO: Rapid protein mechanical strength prediction with an end-to-end deep learning model. *Extreme Mechanics Letters*, 55, p.101803.
9. Yang, Y., Song, Z., Lu, G., Zhang, Q., Zhang, B., [Ni, B.](#), Wang, C., Li, X., Gu, L., Xie, X. and Gao, H., 2021. Intrinsic toughening and stable crack propagation in hexagonal boron nitride. *Nature*, 594(7861), pp.57-61.
10. [Ni, B.](#) and Gao, H., 2020. Engineer energy dissipation in 3D graphene nanolattice via reversible snap-through instability. *Journal of Applied Mechanics*, 87(3), p.031012. [\[demo\]](#)
11. Guo, K. \*, [Ni, B.](#) \* and Gao, H., 2020. Tuning crack-inclusion interaction with an applied T-stress. *International Journal of Fracture*, 222(1-2), pp.13-23. (\*Co-first authors)
12. [Ni, B.](#) and Gao, H., 2021. A deep learning approach to the inverse problem of modulus identification in elasticity. *MRS Bulletin*, 46, pp.19-25. [\[interview\]](#)
13. Li, J., [Ni, B.](#), Zhang, T. and Gao, H., 2018. Phase field crystal modeling of grain boundary structures and growth in polycrystalline graphene. *Journal of the Mechanics and Physics of Solids*, 120, pp.36-48.
14. Hacobian, E.F. \*, Yang, Y. \*, [Ni, B.](#) \*, Li, Y., Li, X., Chen, Q., Guo, H., Tour, J.M., Gao, H. and Lou, J., 2018. Toughening graphene by integrating carbon nanotubes. *ACS nano*, 12(8), pp.7901-7910. (\*Co-first authors) (Highlighted by Rice News [\[website\]](#))

### **Reviews and previews**

15. Luu, R. K., Arevalo, S., Lu, W., [Ni, B.](#), Yang, Z., Shen, S. C., Berkovich, J., Hsu, Y.-C., Zan, S., & Buehler, M. J. (2024). Learning from Nature to Achieve Material Sustainability: Generative AI for Rigorous Bio-inspired Materials Design. *An MIT Exploration of Generative AI*, March.
16. [Ni, B.](#) \*, Steinbach, D. \*, Yang, Z., Lew, A., Zhang, B., Fang, Q., Buehler, M.J. and Lou, J., 2022. Fracture at the two-dimensional limit. *MRS Bulletin*, 47(8), pp.848-862. (\*Co-first authors)
17. [Ni, B.](#) and Gao, H., 2021. Breaking two-dimensional polymeric crystals. *Matter*, 4(3), pp.763-765.
18. [Ni, B.](#) and Gao, H., 2020. Harness the power of fracture: controlled fragmentation of graphene via substrate necking. *Matter*, 2(3), pp.521-524.

### **Book Chapter**

19. [Ni, B.](#) \*, Zhang, T. \*, Li, J., Li, X., and Gao, H., 2019. Topological design of graphene. *Handbook of Graphene*, Volume 2: Physics, Chemistry, and Biology (2019): 1. DOI: 10.1002/9781119468455.ch19 (\*Co-first authors)

### **FUNDING & PROPOSAL EXPERIENCE**

- Assisted the Ph.D. advisor with preliminary work and proposal writing for the application of **National Science Foundation (NSF)** Award #1634492, entitled *topological design of tough multi-functional 2D materials*.
- Assisted the postdoc PI, Prof. Buehler, to prepare a research proposal entitled *atomistic insights into fracture propagation in mixed 2D vertical layered heterostructures*, which had been submitted to **NSF**.
- Co-developed with the current postdoc PI, Prof. Taheri-Mousavi, the proposal on generative AI for

alloy design for winning two joint projects between CMU and **Naval Nuclear Laboratory** with funding of \$1 million per year.

- Near-term targets: NSF CAREER/DMREF; Mid-term: DoD YIP/ONR/AFOSR; Later: DOE AI-for-Science/MURI.

## TALKS AND POSTER PRESENTATIONS

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1. Ni, B., ForceGen: End-to-end de novo protein generation based on nonlinear mechanical unfolding responses using a language diffusion model (oral), ***Society of Engineering Science (SES) Annual Technical Meeting***, Atlanta, GA, USA, 2025
2. Ni, B., Engineer complex materials by merging mechanics with generative AI: a generative mechanics approach (Future Faculty Symposium), ***Society of Engineering Science (SES) Annual Technical Meeting***, Atlanta, GA, USA, 2025
3. Ni, B., and Taheri-Mousavi, S.M., AlloyGPT: forward prediction and inverse design of additively manufacturable alloys via autoregressive language models (poster), ***Gordon Research Conference (GRC) on Metallurgy to Enable Next Generation Engineering***, Stonehill College, MA, USA, 2025
4. Ni, B. and Taheri-Mousavi, S.M., Towards automatic alloy design via large language model powered multi-agent collaborations (oral), ***The 154<sup>th</sup> Annual Meeting & Exhibition of the Minerals, Metals & Materials Society (TMS)***, Las Vegas, NV, USA, 2025
5. Ni, B., Glaser, B. and Taheri-Mousavi, S.M., Forward prediction and inverse design of additively manufacturable alloys via autoregressive language models (poster), ***The 154<sup>th</sup> Annual Meeting & Exhibition of the Minerals, Metals & Materials Society (TMS)***, Las Vegas, NV, USA, 2025
6. Ni, B., Kaplan, D. and Buehler, M., ForceGen—End-to-End De Novo Protein Generation Based on Nonlinear Mechanical Unfolding Responses Using a Language Diffusion Model (oral), ***Materials Research Society (MRS) Fall Meeting***, Boston, MA, USA, 2024
7. Ni, B., Glaser, B. and Taheri-Mousavi, S.M., Forward prediction and inverse design of additively manufacturable alloys via autoregressive language models (oral), ***The Materials Science & Technology (MS&T) technical meeting and exhibition***, Pittsburgh, PA, USA, 2024
8. Ni, B. and Taheri-Mousavi, S.M., Towards automatic alloy design via large language model powered multi-agent collaborations (oral), ***The Materials Science & Technology (MS&T) technical meeting and exhibition***, Pittsburgh, PA, USA, 2024
9. Ni, B., Kaplan, D. and Buehler, M., Generative design of de novo proteins based on secondary-structure constraints using an attention-based diffusion model (oral), ***Society of Engineering Science (SES) Annual Technical Meeting***, Minnesota, MN, USA, 2023
10. Ni, B., Kaplan, D. and Buehler, M., Generative design of de novo proteins based on secondary-structure constraints using an attention-based diffusion model (poster), ***Gordon Research Conference (GRC) on Silk Proteins and the Transition to Biotechnologies***, Smithfield, RI, USA, 2023
11. Ni, B. and Buehler, M., End-to-end ProteinPerceiver to predict secondary protein structures and application to structural proteins (oral), ***Society of Engineering Science (SES) Annual Technical Meeting***, College Station, TX, USA, 2022
12. Ni, B. and Gao, H., Understanding lap shear tests of bilayer graphene via van der Waals interfacial dislocations (oral), ***Society of Engineering Science (SES) Annual Technical Meeting***, College Station, TX, USA, 2022
13. Liu, F., Ni, B. and Buehler, M., Rapid protein mechanical strength prediction with an end-to-end deep learning model (oral), ***Society of Engineering Science (SES) Annual Technical Meeting***, College Station, TX, USA, 2022
14. Ni, B. and Gao, H., Crack evolution in multilayered 2D materials in the presence of interlayer sliding

- (oral), *19th U.S. National Congress on Theoretical and Applied Mechanics*, Austin, TX, USA, 2022
15. Ni, B. and Gao, H., A deep learning approach to the inverse problem of modulus identification in elasticity (oral), *Materials Research Society Fall Meeting*, virtual meeting, 2021
  16. Ni, B., A deep learning approach to the inverse problem of modulus identification in elasticity (oral), *44th Annual Meeting of the Adhesion Society (AS)*, virtual meeting, 2021
  17. Ni, B. and Gao, H., Topological toughening of graphene and other 2D materials (poster), *Aspen center for physics winter conference: low-dimensional solids in hard and soft condensed matter: mechanics, thermodynamics and electrons*, Aspen, CO, USA, 2020
  18. Ni, B. and Gao, H., Topological toughening of graphene and other 2D materials (oral), *Society of Engineering Science (SES) Annual Technical Meeting*, St. Louis, MO, USA, 2019
  19. Ni, B., Guo, K. and Gao, H., Effect of an applied T-stress on crack interaction with inclusions (oral), *Society of Engineering Science (SES) Annual Technical Meeting*, St. Louis, MO, USA, 2019
  20. Ni, B., Guo, K. and Gao, H., Tuning crack-inclusion interaction through T-stress (poster), *Engineering mechanics institute conference (EMI)*, Pasadena, CA, USA, 2019
  21. Ni, B., Li, J., Zhang, T. and Gao, H., Topological toughening of graphene and other 2D materials (oral), *18th National Congress for Theoretical and Applied Mechanics (USNC-TAM)*, Chicago, IL, USA, 2018
  22. Li, J., Ni, B., Zhang, T. and Gao, H., Phase field crystal model for construction of grain boundary in 2D materials (oral), *18th National Congress for Theoretical and Applied Mechanics (USNC-TAM)*, Chicago, IL, USA, 2018
  23. Ni, B. and Gao, H., Topological design of 3D architected sp<sup>2</sup>-bonded carbon assembly: case studies on stiffness, strength and multi-stability (oral), *Society of Engineering Science (SES) Annual Technical Meeting*, Boston, MA, USA, 2017
  24. Ni, B. and Gao, H., Topological toughening of graphene and other 2D materials (oral), *American vacuum society (AVS) 64th International Symposium & Exhibition*, Tampa, FL, USA, 2017
  25. Ni, B., Atomic modeling of toughening graphene through bio-inspired topological designs (poster), *Society of Engineering Science (SES) Annual Technical Meeting*, Maryland, MD, USA, 2016

## HONORS AND AWARDS

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- Travel award, 2<sup>nd</sup> **Future Faculty** Symposium at SES annual meeting Oct 2025
- **Rising Star** in Materials Science and Engineering (MSE) Oct 2023  
Awarded by CMU, MIT and Stanford University as “an endorsement of one’s potential as a leader in MSE”.
- Travel award, 1<sup>st</sup> **Future Faculty** Symposium at SES annual meeting Oct 2023
- Travel award, Aspen center for physics 2020 winter conference Feb 2020
- Student travel award, 2D materials Focus topic, American Vacuum Society (AVS)-64 international symposium Nov 2017
- The Scholarship in the name of *Tang Zhaoqian*, XJTU, China 2011
- National Scholarship for Encouragement, XJTU, China 2010
- National Scholarship, XJTU, China 2009
- National Scholarship, XJTU, China 2008
- The First Prize, Competition of Fundamental Mechanics, Shaanxi Province, China 2008

## TEACHING EXPERIENCE

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### Guest lecturer, CMU

- 27-537 *Data Analytics for Materials Science* by Prof. Mohadeseh Taheri-Mousavi Spring 2025

### Teaching Assistant/Guest lecturer, MIT

- 3.021 *Intro to Modeling & Simulation* by Profs. Markus Buehler & Rodrigo Freitas Spring 2023
- 1.545 *Atomistic Modeling and Simulation: Mat and Struct* by Prof. Markus Buehler Fall 2022
- 1.021 *Intro to Modeling & Simulation* by Profs. Markus Buehler & Rodrigo Freitas Spring 2022

### Teaching Assistant, Brown University

- ENGN 1750: Advanced Mechanics of Solids by Prof. Allan Bower Fall 2018
- ENGN 1300: Structural Analysis by Prof. Huajian Gao Spring 2018
- ENGN 2410: Thermodynamics of Materials by Prof. David Paine Fall 2017

## ADVISING AND MENTORING EXPERIENCE

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Advisee: **Frank J. Liu**, Newton South High School Summer 2021-Spring 2022

- I served as the acting mentor for Frank when he attended Research Science Institute (RSI) at MIT and provided him with continuous guidance during our latter joint research project. Frank is named in Top 5 oral presentation speakers (among 18) and the Regeneron Science Talent search Top 300 scholars in 2021 [[link](#)]. Our work was published later on *Extreme Mechanics Letters* in 2022.

Advisee: **Jessica Zheng**, South Brunswick High School Summer 2022

Advisee: **Grace Choi**, Bloomington High School South Summer 2023

- With Yiwen Hu, I served as co-mentor for Jessica and Grace when they joined RSI at MIT in 2022 and 2023 and assisted their research projects on proteins and cellular agriculture during the periods.

Advisee: **Zhiyang An**, undergraduate, CMU Spring 2024 - present

- I serve as the research mentor for Ziyang on an ongoing research project of applying DL to understand the strength of tungsten-based alloys. Zhiyang successfully presented our preliminary result at *MS&T* 2024 meeting.

Advisee: **Jixuan Dong**, Ph.D. candidate, CMU Spring 2025 - present

Advisee: **Hasan Jame**, Ph.D. candidate, CMU Spring 2025 - present

- I serve as the research mentor for them on developing augmentations for AlloyGPT models targeting uncertainty quantification and gradient alloy design.

## PROFESSIONAL ACTIVITIES

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**Reviewer (journals):** Physical Review Letters (PRL), Proceedings of the National Academy of Sciences of the United States of America (PNAS), Journal of the Mechanics and Physics of Solids (JMPS), Physical Review B (PRB), Carbon, Modeling and Simulation in Materials Science and Engineering (MSMSE), Journal of Materials Research (JMR), MRS Bulletin (MRSB), Mechanics of Materials (MM), Journal of

the Mechanical Behavior of Biomedical Materials (JMBBM), ACS Applied Nano Materials.

**Guest editor:** Biomimetics — Special Issue: “Generative Biomimetics: AI-Driven Exploration of Materials and Molecular Architectures.”

## REFERENCES

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**Prof. Huajian Gao** (Ph.D. advisor)

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**Prof. Jun Lou** (Ph.D. thesis committee member and collaborator)

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**Prof. Mohadeseh Taheri-Mousavi** (current postdoc supervisor)

Assistant Professor, Materials Science and Engineering

Carnegie Mellon University

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