

Gang Seob Jung
Research Staff
Computational Science & Engineering Division (CSED)
Oak Ridge National Laboratory (ORNL)
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EDUCATION

- Doctor of Philosophy** in Civil & Environmental Engineering (GPA 4.9/5.0) 09/2013- 06/2019
Massachusetts Institute of Technology, Department of CEE (Cambridge, U.S.)
ADVISOR: Markus J. Buehler
- Master of Science** in Physics (GPA 3.9/4.0) 04/2006 - 03/2008
The University of Tokyo, Department of Physics (Tokyo, Japan)
ADVISOR: Shinji Tsuneyuki
- Bachelor of Science** in Physics, (GPA 3.9/4.0, graduation with first prize) 04/2002 - 03/2006
University of Tsukuba, College of Natural Science (Tsukuba, Japan)

RESEARCH EXPERTISE

Multiscale modeling based on atomistic models combined with **Artificial Intelligence (AI)/Machine Learning (ML)** and **High-Performance Computing (HPC)** to understand the **materials synthesis process, interaction between different phases, microstructure evolution, mechanical failure, and structure-property relation** from micro- to macro-scales.

DISTINGUISHED STAFF (WIGNER) FELLOWSHIP (2019-2022)

Distinguished research project in the area of: "Multiscale Computational Methodologies for Materials Properties/Processes"

PROFESSIONAL EXPERIENCE

- Research Staff, CSED, ORNL, US** 2022-Now
Atomistic Models for Materials Degradation through Enzyme (PI) 2024-Now
Active Learning of Atomistic Surrogate Models for Rare Event (PI) 2023
- Distinguished Staff (Wigner) Fellowship, CSED, ORNL, US** 2019-2022
Multiscale Computational Methodologies for Materials Properties/Processes (PI) 2019-2022
- Postdoctoral Research Associate, CEE, MIT, US** (Advisor: Markus J. Buehler) 2019
- Graduate Research Assistant, CEE, MIT, US** (Advisor: Markus J. Buehler) 2013-2019
Foldable and adaptive two-dimensional electronics MURI (AFOSR)
Models to predict biomaterials performance (NIH)
- Researcher, KISTI, Daejeon, Korea** 2011-2013
Development of MM_PAR, C++ code for classical MD with MPI/OpenMP
High-performance computing
- Research Engineer, LG DISPLAY, Paju, Korea** (military service) 2008-2011
Touch panel embedded in LCD: FEM simulations and Experimental analysis
- Graduate Research Assistant, Physics, Tokyo University** (Advisor: Shinji Tsuneyuki) 2006-2008
Free energy calculations with extended ensemble methods

HONORS & AWARDS

- R&D 100 Finalists (BIPHASICS, ORNL)** 2025
- Japan-Korea Joint Government Scholarship** 2001 - 2006
- University of Tokyo Fellowship** 2006 - 2008
- LG DISPLAY Industrial Scholarship** 2007 - 2008
- MIT Presidential Graduate Fellowship (Edward H. Linde)** 2013 - 2014
- ORNL Distinguished Staff Fellowship (Eugene Wigner)** 2019 - 2022
- The First Prize (Physics), University of Tsukuba** 2006

PUBLICATIONS (*Co-first author, †Corresponding author), **Google +2900 (h-index 27, i10-index 40)**

46. B Haberl†, M Guthrie, **GS Jung**, LB Bayu Aji, JJ Molaison, S Irle, JE Bradby, A pressure-driven amorphous-crystalline transition reveals the metastability of silicon and germanium, *Materials Today*, **2025**
45. A Wiechert, **GS Jung**, D Stamberga, GG Jang, MJ Cordon, R Custelcean, D Sholl, C Tsouris†, Biphasic Solvents for Post-Combustion CO₂ Capture from Natural Gas Flue Gas, *Chemical Engineering Journal*, **2025**
44. **GS Jung**†, Atomic Energy Accuracy of Neural Network Potentials: harnessing Pretraining and Transfer Learning, *Journal of Chemical Information and Modeling*, **2025**
43. V Bocharova†, E Druvva, J Cahill, I Popov, I Dishner, M Zhou, **GS Jung**, A Ullman, D Carper, J Damron, J Keum, C Gainaru, S Chen, J Foster, J Michener, Factors Modulating the Hydrolysis of Nylon-6,6 by a Nylon Hydrolase Enzyme, *Polymer Chemistry*, **2025**
42. GH Ryu†, **GS Jung**†, J Warner†, Atomic Scale Dynamic Mechanisms of Embedded MoS₂ Wires, *ACS Nano*, **2024**
41. **GS Jung**†, Enhancing High-Fidelity Neural Network Potentials through Low-Fidelity Sampling, *APL Machine Learning*, **2024**
40. **GS Jung**†, P Yoo, MR Ryder, F Vautard, A Annamraju, S Irle, N Gallego, E Lara-Curzio, Molecular Origin of Viscoelasticity and Influence of Methylation in Mesophase Pitch, *Carbon*, **2024**
39. P Yoo, **GS Jung**, MR Ryder, F Vautard, E Cakmak, S Wi, MC Weisenberger, E Lara-Curzio, JP Mathews†, S Irle†, Large-scale atomistic model construction of subbituminous and bituminous coals for solvent extraction simulations with reactive molecular dynamics, *Carbon*, **2024**
38. GG Jang, **GS Jung**, A Meyer, A Kasturi, D Stamberga, R Custelcean, C Tsouris†, Effective Direct Steam Regeneration of Solid Sorbent Used for Carbon Capture, *Chemical Engineering Journal*, **2024**
37. A Annamraju†, **GS Jung**†, S Bhagia, J Damron, MR Ryder, MA Arnould, E Cakmak, RM Paul, F Vautard, S Irle, N Gallego, E Lara-Curzio, On the Role of Methyl Groups in Molecular Architecture of Mesophase Pitches, *Fuel*, **2024**.
36. GG Jang†, **GS Jung**, J Seo, JK Keum, M Yoon, J Damron, AK Naskar, R Custelcean, A Kasturi, S Yiacoumi, C Tsouris, Tailoring chemical absorption-precipitation to lower the regeneration energy for CO₂ capture solvent, *ChemSusChem*, **2024**
35. **GS Jung**†, JY Choi, SM Lee, Active Learning of Neural Network Potentials for Rare Events, *Digital Discovery*, **2024**
34. **GS Jung**†, Y Yoshimoto, KJ Oh, S Tsuneyuki†, Extended ensemble molecular dynamics for thermodynamics of phases, *arXiv preprint arXiv:2308.08098*, **2023**
33. **GS Jung**†, HJ Myung, S Irle, Artificial Neural Network Potentials for Mechanics and Fracture Dynamics of Two-Dimensional Crystals, *Machine Learning: Science and Technology*, **2023**
32. J Jhu*, J-H Park*, SA Vitale, W Ge, **GS Jung**, J Wang, M Mohamed, T Zhang, M Ashok, M Xue, X Zheng, Z Wang, J Hansryd, A Chandrakasn, J Kong†, T Palacios†, Low thermal budget synthesis of monolayer molybdenum disulfide for silicon back-end-of-line integration on 200 mm platform, *Nature Nanotechnology*, **2023**. [MIT News \(April 27,2023\)](#)
31. ML Pasini†, **GS Jung**, S Irle, Graph Neural Network Predict Energetic and Mechanical Properties for Models of Solid Solution Metal Alloy Phases, *Computational Materials Science*, **2023**
30. H Park, **GS Jung**, Y Lu, K-L Tai, KM Ibrahim, JH Warner†. Atomic Scale Insights into the Lateral and Vertical Epitaxial Growth in Two-Dimensional Pd₂Se₃-MoS₂ Heterostructures. *ACS Nano*, **2022**
29. W Xu, **GS Jung**, S Zhang, ATS Wee, JH Warner†. Atomically sharp jagged edges of chemical vapor deposition grown WS₂ for electrocatalysis. *Materials Today Nano*, **2022**
28. **GS Jung**†, S Irle, Bobby Sumpter, Dynamic Aspects of Graphene Deformation and Fracture, *Carbon*, **2022**
27. H Wang*, Z Yao*, **GS Jung**, O Song, M Hempel, T Palacios, G Chen, MJ Buehler, Aspuru-Guzik, J Kong†, Realizing Frank-van der Merwe Growth in Bilayer Graphene. *Matter*, **2021**

26. Y Yu*, **GS Jung***, C Liu, C M Rouleau, M Yoon, G Eres, Duscher, K Xiao, S Irle, A Puzos, D Geohegan, Strain-Induced Growth of Twisted Bilayers during the Coalescence of Monolayer MoS₂ Crystals. *ACS Nano*, **2021**
25. GH Ryu[†]*, **GS Jung[†]***, HJ Park, RJ Chang, JH Warner[†], Atomistic Mechanics of Torn Back Folded Edges of Triangular Voids in Monolayer WS₂. *Small*, **2021**
24. M Milazzo, A David, **GS Jung**, S Danti, and MJ Buehler[†], Molecular origin of viscoelasticity in mineralized collagen fibrils. *Biomaterials Science*, **2021**
23. Q Qian*, R Zu*, Q Ji, **GS Jung**, K Zhang, Y Zhang, MJ Buehler, J Kong, V Gopalan, and S Huang[†], Chirality-Dependent Second Harmonic Generation of MoS₂ Nanoscroll with Enhanced Efficiency. *ACS Nano*, **2020**
22. I Su, **GS Jung**, N Narayanan, MJ Buehler[†], Perspective on Three-Dimensional Printing of Self-Assembling Materials and Structures. *Current Opinion in Biomedical Engineering*, **2020**. 15, 59-67.
21. JL Zitnay, **GS Jung**, A Lin, Z Qin, Y Li, SM Yu, MJ Buehler, JA Weiss[†], Accumulation of collagen molecular unfolding is the mechanism of cyclic fatigue damage and failure in collagenous tissues. *Science Advances*, **2020**
20. M Milazzo, **GS Jung**, S Danti, and MJ Buehler[†], Mechanics of mineralized collagen fibrils upon transient load. *ACS Nano*, **2020**. 14, 7, 8307-8316.
19. J Yeo*, Y Qiu*, **GS Jung**, Y-W Zhang, MJ Buehler[†], and DL Kaplan[†], Adverse effects of Alport syndrome-related missense mutations on collagen IV: unified insights from molecular dynamics simulations and experiments. *Biomaterials*, **2020**. 240, 119857.
18. M Milazzo, **GS Jung**, S Danti, and MJ Buehler[†], Wave propagation and energy dissipation in collagen molecule. *ACS Biomaterials Science & Engineering*, **2020**. 6, 3, 1367-1374.
17. J Chen, **GS Jung**, GH Ryu, RJ Chang, S Zhou, Y Wen, MJ Buehler, and JH Warner[†], Atomically Sharp Dual Grain Boundaries in 2D WS₂ Bilayers. *Small*, **2019**. 30, 1902590.
16. E Beniash, CA Stiffler, C-Y Sun, **GS Jung**, Z Qin, MJ Buehler[†], PUPA Gilbert[†]. The hidden structure of human enamel. *Nature Communications*, **2019**. 10, 4383
15. **GS Jung***, S Wang*, Z Qin, S Zhou, M Danaie, AI Kirkland, MJ Buehler[†], JH Warner[†], Anisotropic Fracture Dynamics Due to Local Lattice Distortions. *ACS Nano*, **2019**. 13, 5693-5702.
14. Y Zhou, SG Sarwat, **GS Jung**, MJ Buehler, H Bhaskaran, and JH Warner[†], Grain Boundaries as Electrical Conduction Channels in Polycrystalline Monolayer WS₂. *ACS Applied Materials & Interfaces*, **2019**. 11, 10189.
13. J Yeo*, **GS Jung***, FJ Martin-Martinez*, J Beem, Z Qin, MJ Buehler[†]. Multiscale design of graphyne materials, from atom to structure. *Advanced Materials*, **2019**. 1805660
12. **GS Jung**, MJ Buehler[†]. Atomic-scale hardening mechanisms apply on larger scales in architected materials. *Nature*, **2019**. 565, 303-304
11. **GS Jung**, MJ Buehler[†]. Multiscale Mechanics of Triply Periodic Minimal Surfaces of Three-Dimensional Graphene Foams. *Nano Letters*, **2018**. 18, 4845-4852
10. J Yeo, **GS Jung**, FJ Martin-Martinez, S Ling, GX Gu, Z Qin, MJ Buehler[†]. Materials-by-Design: Computation, Synthesis, and Characterization from Atoms to Structures. *Physica Scripta*, **2018**, 93, 053003.
9. J Yeo, **GS Jung**, A Tarakanova, FJ Martín-Martínez, Z Qin, Y Cheng, Y-W Zhang, and MJ Buehler[†], Multiscale modeling of keratin, collagen, elastin and related human diseases: Perspectives from atomistic to coarse-grained molecular dynamics simulations. *Extreme Mechanics Letters*, **2018**, 20, 112-124.
8. **GS Jung***, S Wang*, Z Qin, FJ Martin-Martinez, JH. Warner[†] and MJ Buehler[†]. Interlocking friction governs mechanical fracture of bilayer MoS₂. *ACS Nano*, **2018**, 10, 3600-3608.
7. Y Han*, MY Li*, **GS Jung***, MA Marsalis, Z Qin, MJ Buehler, LJ Li[†] and DA Muller[†], Sub-nanometre channels embedded in two-dimensional materials. *Nature Materials*, **2018**, 17, 129-133 (Feb. 2018 COVER Article) [MIT News \(Dec 7, 2017\)](#)
6. **GS Jung**, MJ Buehler[†]. Multiscale Modeling of Muscular-Skeletal Systems. *Annual Review Biomedical Engineering*, **2017**, 19, 435-57

5. **GS Jung**, J Yeo, Z Tian, Z Qin, MJ Buehler[†]. Unusually low and density-insensitive thermal conductivity of three-dimensional gyroid graphene. *Nanoscale*, **2017**, 9, 13477-13484
4. Z Qin*, **GS Jung***, MJ Kang, MJ Buehler[†]. The mechanics and design of a lightweight three-dimensional graphene assembly. *Science Advances*, **2017**, 3, e1601536, [MIT News \(Jan 6, 2017\)](#), [CNN News \(Jan 13, 2017\)](#), [Materialstoday \(Jan, 12,2017\)](#), [Discovery's Seeker \(Jan 6, 2017\)](#)
3. C-T Chen, FJ Martin-Martinez, **GS Jung**, MJ Buehler[†]. Polydopamine and eumelanin molecular structures investigated with ab-initio calculations. *Chemical Science*, **2016**, 8, 1631-41
2. S Wang*, Z Qin*, **GS Jung**, FJ Martin-Martinez, K Zhang, JH Warner[†] and MJ Buehler[†]. Atomically Sharp Crack Tips in Monolayer MoS₂ and Their Enhanced Toughness by Vacancy Defects. *ACS Nano*, **2016**, 10, 9831-9, [NanoTechWeb News](#)
1. **GS Jung**, Z Qin, MJ Buehler[†]. Molecular mechanics of polycrystalline graphene with enhanced fracture toughness. *Extreme Mechanics Letters*, **2015**, 2, 52-9, [CEE@MIT News in Brief](#)

BOOK CHAPTERS

2. Z Qin, **GS Jung**, FJ Martin-Martinez, MJ Buehler[†], Multiscale Modeling and Applications of Bioinspire Materials with Gyroid Structures. *Computational Materials, Chemistry and Biochemistry: From Bold initiatives to the Last Mile*, **2021**
1. **GS Jung**, Z Qin, MJ Buehler[†]. Mechanical Properties and Failure of Biopolymers: Atomistic Reactions to Macroscale Response. In *Polymer Mechanochemistry*, ed. R Boulatov, 369:317-43: Springer International Publishing. *Topics in Current Chemistry*, **2015**, 317-43

THESIS

- Title: Extended ensemble molecular dynamics for predicting a material structure** **2008**
 Master of Science in Physics (**The University of Tokyo**), Advisor: Shinji Tsuneyuki
- Title: Multiscale modeling of two-dimensional materials: structure, properties, and designs** **2019**
 Doctor of Philosophy in Civil & Environmental Engineering (**MIT**), Advisor: Markus J. Buehler

CONFERENCES & WORKSHOPS & TALKS

14. **GS Jung**, "Neural Network Potentials: Challenges and Future Directions", Workshop, University of Connecticut, April 2, 2024
13. **GS Jung**, "Data Sampling and Distillation for Neural Network Potentials", Invited Talk, University of Connecticut, Feb 16, 2024
12. **GS Jung**, S Lee, JY Choi, "Data Distillation for Neural Network Potentials toward Foundational Dataset", NeurIPS 2023, December 15, 2023, New Orleans.
11. **GS Jung** "Active Learning of Atomistic Surrogate Models for Rare Events", Invited Talk, University of Kentucky, April 11, 2023
10. **GS Jung** "Multiscale Modeling of Two-Dimensional Materials for Fracture and Crystal Growth", Lawrence Berkeley National Laboratory, May 22, 2019
9. **GS Jung**, MJ Buehler, "Multiscale Mechanics of triply periodic minimal surfaces of three-dimensional graphene foams", Multifunctional Materials Workshop, US-Army-Natick Lab, Nov 29, 2018
8. **GS Jung**, MJ Buehler, "Mechanics of Triply Periodic Minimal Surfaces of Three-Dimensional Graphene Foams" Materials Research Society (MRS), 2018 Fall Meeting, 2018
7. **GS Jung**, MJ Buehler, "Molecular mechanics of MoS₂ monolayer with point defect and grain boundary" Materials Research Society (MRS), 2018 Fall Meeting, 2018

6. **GS Jung**, MJ Buehler, "Thermal conductivity of triply periodic minimal surface of three-dimensional graphene foams" Materials Research Society (MRS), Fall Meeting, 2018
5. **GS Jung**, S Wang, Z Qin, J Warner, MJ Buehler, "Single Atomic Deformation Regulate the Fracture Dynamics and Strength" MIT-MRL Symposium, Cambridge, 2018
4. Z Qin, **GS Jung**, S Wang, Martin-Martinez FJ, J Warner, Buehler MJ, "Computational modeling of the mechanics and fracture of 2D materials with defects and grain boundaries" 14th International Conference on Fracture, 2017
3. Martin-Martinez FJ, Z Qin, JJ Yeo, **GS Jung**, Buehler MJ, "Multiscale Modeling of Nanomaterials: DFT and MD simulations" 253rd ACS National Meeting & Exposition, April 4, 2017
2. Z Qin, **GS Jung**, S Wang, FJ Martin-Martinez, J Warner, MJ Buehler, "Mechanics and Fracture of 2D Materials with Defects and Grain Boundaries" AVS 63rd International Symposium & Exhibition, November 6, 2016
1. **GS Jung**, Z Qin, MJ Buehler, "Enhanced Fracture Toughness of Polycrystalline Graphene" Materials Research Society (MRS), Fall Meeting, 2015

SOFTWARE

1. **GS Jung**, JY Choi, SM Lee, AL-ASMR: Active Learning of Atomistic Surrogate Models for Rare Events, ORNL 2023. <https://doi.org/10.11578/dc.20230823.1>

TUTORIAL

1. **Neural Network Potential Training**, <https://github.com/gsjung0419/TorchANITutorials>

PATENTS & APPLICATIONS

7. Application #: 63/710,082, "Diethylenetriamine based Biphasic Absorbent for Post-Combustion Carbon Dioxide Capture", Filed Date: 10/22/2024, Status: Application.
6. Application #: 19/027,854, "Solid CO₂-diamine-NaCl molecular complex for low-energy CO₂ regeneration", Filed Date: 01/17/2025, US 2025/023587 A1
5. **GS Jung**, SS Hwang, YJ Yi, JH Lee, Touch panel and liquid crystal display device including the same. US Patent 8,970,509
4. SC An, CS Kim, SS Hwang, **GS Jung**, Touch panel and method for manufacturing the same. US Patent 8,947,370
3. SC An, HK Kang, SS Hwang, **GS Jung**, Touchscreen panel. US Patent 8,970,508
2. **GS Jung**, HK Kang, SC An, SS Hwang, Electrostatic capacity type touch screen panel and method of manufacturing the same. US Patent 8,780,061
1. SS Hwang, **GS Jung**, JY Lee, SJ Yoo, Touchscreen panel. US Patent 8,493,349

SCIENTIFIC REVIEWER WORK

JMBBM, Carbon, MRS Bulletin, Nanomaterials, Molecule, Materials Today Advances, PNAS, Cell Reports Physical Science, ACS Nanomaterials, ACS Omega, Physical Review Letter, Crystals, Carbon Trend, Journal of Physical Chemistry C, ACS Biomaterials Science & Engineering, Nanotechnology, Physical Review Materials, Journal of Physics: Materials, Molecular Simulation, Digital Discovery.