

**Gang Seob Jung**  
Eugene Wigner Fellow  
Computational Science & Engineering Division (CSED)  
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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 INTEREST

Understanding the **materials synthesis process**, **interaction between different phases**, **microstructure evolution**, **mechanical failure**, and **structure-property relation** from micro- to macro-scales by utilizing **computational modeling** based on multiscale and multiphysics paradigms.

## RESEARCH PROJECT

**Wigner Fellowship Project:** "Development of integrated multiscale fluid-solid interface models for the predictive design of energy and water processes".

## PROFESSIONAL EXPERIENCE

- Eugene Wigner Fellow, CSED, ORNL, US** (Advisor: Stephan Irle) 2019-Now
- 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

- 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 - Now
- The First Prize (Physics), University of Tsukuba** 2006

## TEACHING and MENTORING

- Teaching Assistant, Physics, University of Tokyo, Japan** 2007
- Research Mentor for MIT CEE Undergraduate Research Opportunity Program** 2016-2018
- Research Mentor for Research Scholar Institute (RSI) for K-12 students** 2015

## **PUBLICATIONS** (\*Co-first author, †Corresponding author), **Google Citation +500**

25. M Milazzo, **GS Jung**, S Danti, and MJ Buehler<sup>†</sup>, Wave propagation and energy dissipation in collagen molecule. *in submission*
24. **GS Jung**, JH Warner, and MJ Buehler<sup>†</sup>, Fracture and Crack Propagation: Recent Progress in Computational Modeling and Experiments. *in preparation*
23. H Wang\*, WS Leong\*, Z Yao\*, **GS Jung**, O Song, M Hempel, T Palacios, G Chen, MJ Buehler, A Aspuru-Guzik, J Kong<sup>†</sup>, Realizing Frank-van der Merwe Growth in Bilayer Graphene. *in revision*
22. J Chen, **GS Jung**, GH Ryu, RJ Chang, S Zhou, Y Wen, MJ Buehler, and JH Warner<sup>†</sup>, Atomically Sharp Dual Grain Boundaries in 2D WS<sub>2</sub> Bilayers. *Small*, **2019**. 30, 1902590.
21. Y Zhou, SG Sarwat, **GS Jung**, MJ Buehler, H Bhaskaran, and JH Warner<sup>†</sup>, Grain Boundaries as Electrical Conduction Channels in Polycrystalline Monolayer WS<sub>2</sub>. *ACS Applied Materials & Interfaces*, **2019**. 11, 10189.
20. J Yeo\*, Y Qiu\*, **GS Jung**, Y-W Zhang, MJ Buehler<sup>†</sup>, and DL Kaplan<sup>†</sup>, Adverse effects of Alport syndrome-related missense mutations on collagen IV: unified insights from molecular dynamics simulations and experiments. *In revision*
19. **GS Jung**, MJ Buehler<sup>†</sup>. Hierarchical Designs of Lightweight and Tough Structures with Triply Periodic Minimal Surfaces. *in preparation*
18. **GS Jung**, JH Warner, MJ Buehler<sup>†</sup>. Mechanics of MoS<sub>2</sub> Monolayer with Point Defects and Grain Boundaries. *in preparation*
17. JL Zitnay, **GS Jung**, A Lin, Z Qin, Y Li, SM Yu, MJ Buehler, JA Weiss<sup>†</sup>, Progressive molecular failure of collagen as a mechanism of tendon fatigue. *in submission*
16. **GS Jung**\*, S Wang\*, Z Qin, S Zhou, M Danaie, AI Kirkland, MJ Buehler<sup>†</sup>, JH Warner<sup>†</sup>, Propagation Anisotropy Due to Local Lattice Distortions. *ACS Nano*, **2019**. 13, 5693-5702.
15. E Beniash, CA Stiffler, C-Y Sun, **GS Jung**, Z Qin, MJ Buehler<sup>†</sup>, PUPA Gilbert<sup>†</sup>. The hidden structure of human enamel. *Nature Communications*, **2019**. 10, 4383
14. **GS Jung**, MJ Buehler<sup>†</sup>. Atomic-scale hardening mechanisms apply on larger scales in architected materials. *Nature*, **2019**. 565, 303-304
13. J Yeo\*, **GS Jung**\*, FJ Martin-Martinez\*, J Beem, Z Qin, MJ Buehler<sup>†</sup>. Multiscale design of graphyne materials, from atom to structure. *Advanced Materials*, **2019**. 1805660
12. **GS Jung**, MJ Buehler<sup>†</sup>. Multiscale Mechanics of Triply Periodic Minimal Surfaces of Three-Dimensional Graphene Foams. *Nano Letters*, **2018**. 18, 4845-4852
11. J Yeo, **GS Jung**, FJ Martin-Martinez, S Ling, GX Gu, Z Qin, MJ Buehler<sup>†</sup>. Materials-by-Design: Computation, Synthesis, and Characterization from Atoms to Structures. *Physica Scripta*, **2018**, 93, 053003.
10. **GS Jung**\*, S Wang\*, Z Qin, FJ Martin-Martinez, JH. Warner<sup>†</sup> and MJ Buehler<sup>†</sup>. Interlocking friction governs mechanical fracture of bilayer MoS<sub>2</sub>. *ACS Nano*, **2018**, 10, 3600-3608.
9. J Yeo, **GS Jung**, A Tarakanova, FJ Martín-Martínez, Z Qin, Y Cheng, Y-W Zhang, and MJ Buehler<sup>†</sup>, 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. Y Han\*, MY Li\*, **GS Jung**\*, MA Marsalis, Z Qin, MJ Buehler, LJ Li<sup>†</sup> and DA Muller<sup>†</sup>, Sub-nanometre channels embedded in two-dimensional materials. *Nature Materials*, **2018**, 17, 129-133 (Feb. 2018 COVER Article) [MIT News \(Dec 7, 2017\)](#)
7. **GS Jung**, J Yeo, Z Tian, Z Qin, MJ Buehler<sup>†</sup>. Unusually low and density-insensitive thermal conductivity of three-dimensional gyroid graphene. *Nanoscale*, **2017**, 9, 13477-13484
6. **GS Jung**, MJ Buehler<sup>†</sup>. Multiscale Modeling of Muscular-Skeletal Systems. *Annual Review Biomedical Engineering*, **2017**, 19, 435-57

5. Z Qin\*, **GS Jung\***, MJ Kang, MJ Buehler<sup>†</sup>. 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 \(Jan 6, 2017\)](#)
4. C-T Chen, FJ Martin-Martinez, **GS Jung**, MJ Buehler<sup>†</sup>. Polydopamine and eumelanin molecular structures investigated with ab-initio calculations. *Chemical Science*, **2016**, 8, 1631-41
3. S Wang\*, Z Qin\*, **GS Jung**, FJ Martin-Martinez, K Zhang, JH Warner<sup>†</sup> and MJ Buehler<sup>†</sup>. Atomically Sharp Crack Tips in Monolayer MoS<sub>2</sub> and Their Enhanced Toughness by Vacancy Defects. *ACS Nano*, **2016**, 10, 9831-9, [NanoTechWeb News](#)
2. **GS Jung**, Z Qin, MJ Buehler<sup>†</sup>. 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
1. **GS Jung**, Z Qin, MJ Buehler<sup>†</sup>. Molecular mechanics of polycrystalline graphene with enhanced fracture toughness. *Extreme Mechanics Letters*, **2015**, 2, 52-9, [CEE@MIT News in Brief](#)

## 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

8. **GS Jung** "Multiscale Modeling of Two-Dimensional Materials for Fracture and Crystal Growth", Lawrence Berkeley National Laboratory, May 22, 2019
7. **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
6. **GS Jung**, MJ Buehler, "Molecular mechanics of MoS<sub>2</sub> monolayer with point defect and grain boundary" Materials Research Society (MRS), 2018 Fall Meeting, 2018
5. **GS Jung**, MJ Buehler, "Thermal conductivity of triply periodic minimal surface of three-dimensional graphene foams" Materials Research Society (MRS), Fall Meeting, 2018
4. **GS Jung**, S Wang, Z Qin, J Warner, MJ Buehler, "Single Atomic Deformation Regulate the Fracture Dynamics and Strength" MIT-MRL Symposium, Cambridge, 2018
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

## PATENTS

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**

Scientific Reports, Journal of the Mechanical Behavior of Biomedical Materials