

## Education

### Massachusetts Institute of Technology (MIT)

Sep 2017 – May 2023

PhD, Physical Materials Chemistry

NSF Graduate Research Fellowship

Thesis Title: Elucidating Structure-Property Relationships for Targeted Materials Mechanical Design

### University of California, Los Angeles (UCLA)

Sep 2013 – Jun 2017

BS, Materials Science and Engineering – GPA 3.9/4.0

UCLA Engineering Achievement Award for Student Welfare

## Academic Experience

### MIT, Laboratory for Atomistic and Molecular Mechanics - NSF Graduate Research Fellow, PhD Candidate

 Dec 2019 – May 2023

- Leverage AI, atomistic simulations, and experiment for understanding material structure-property relationships
- Probe and predict material properties via molecular dynamics simulation and machine learning surrogate models
- Devise AI workflows for generative design of new materials with specified target behavior

### MIT, Department of Materials Science and Engineering - Graduate Student Researcher

Dec 2017 – Dec 2019

- Design and synthesis of small amphiphilic molecule platform for self-assembly into robust hierarchical materials
- Molecular, nanoscale, and mesoscale characterization of chemical structures, nanoribbons, and centimeter-long assemblies

### UCLA, Department of Materials Science and Engineering - Undergraduate Student Researcher

Jan 2016 – Jun 2017

- Synthesis of iron oxide nanoparticles for application in magnetic hyperthermia drug delivery
- Nanoparticle characterization and incorporation into drug delivery system

## Publications

**Lew, A.J.**, Accelerating Materials Recipe Acquisition via LLM-Mediated Reinforcement Learning. *MRS Advances*. (2025).

<https://doi.org/10.1557/s43580-025-01143-9>

**Lew, A.J.**, A Brief Survey of ML Methods Predicting Molecular Solubility: Towards Lighter Models via Attention and Hyperparameter Optimization. *Preprints*. 2024090849 (2024). <https://doi.org/10.20944/preprints202409.0849.v1>

**Lew, A.J.**, Stifler, C.A., Cantamessa, A., Tits, A., Ruffoni, D., Gilbert, P.U.P.A., Buehler, M.J. Deep learning virtual indenter maps nanoscale hardness rapidly and non-destructively, revealing mechanism and enhancing bioinspired design. *Matter*. (2023). <https://doi.org/10.1016/j.matt.2023.03.031>

**Lew, A.J.**, Stifler, C.A., Tits, A., Schmidt, C.A., Scholl, A., Cantamessa, A., Müller, L., Delaunois, Y., Compère, P., Ruffoni, D., Buehler, M.J., Gilbert, P.U.P.A. A molecular scale understanding of misorientation toughening in corals and seashells. *Advanced Materials*. (2023). <https://doi.org/10.1002/adma.202300373> – **Cover Feature & University of Liège News Feature**

**Lew, A.J.**, Buehler, M.J. Single-shot forward and inverse hierarchical architected materials design for nonlinear mechanical properties using an attention-diffusion model. *Materials Today*. (2023). <https://doi.org/10.1016/j.mattod.2023.03.007> – **Highlighted Paper**

**Lew, A.J.**, Jin, K., Buehler, M.J. Designing architected materials for mechanical compression via simulation, deep learning, and experimentation. *npj Computational Materials*. 9, 80 (2023). <https://doi.org/10.1038/s41524-023-01036-1>

Ni, B., Steinbach, D., Yang, Z., **Lew, A.J.**, Zhang, B., Fang, Q., Buehler, M.J., Lou, J. Fracture at the two-dimensional limit. *Materials Research Society Bulletin*. 47 (2022). <https://doi.org/10.1557/s43577-022-00385-4>

**Lew, A.J.**, Beniash, E., Gilbert, P.U.P.A., Buehler, M.J. Role of the mineral in the self-healing of cracks in human enamel. *ACS Nano*. 16, 7, 10273–10280 (2022). <https://doi.org/10.1021/acsnano.1c10407>

**Lew, A.J.**, Buehler, M.J. DeepBuckle: Extracting physical behavior directly from empirical observation for a material agnostic approach to analyze and predict buckling. *Journal of the Mechanics and Physics of Solids*. 164, 104909 (2022). <https://doi.org/10.1016/j.jmps.2022.104909> – **Patent Application**

**Lew, A.J.**, Buehler, M.J. A deep learning augmented genetic algorithm approach to polycrystalline 2D material fracture discovery and design. *Applied Physics Reviews*. 8, 041414 (2021). <https://doi.org/10.1063/5.0057162> – **Featured Article**

**Lew, A.J.**, Buehler, M.J. Encoding and exploring latent design space of optimal material structures via a VAE-LSTM model. *Forces in Mechanics*. 5, 100054 (2021). <https://doi.org/10.1016/j.finmec.2021.100054>

**Lew, A.J.**, Yu, CH., Hsu, YC., Buehler M.J. Deep learning model to predict fracture mechanisms of graphene. *npj 2D Materials Applications*. 5, 48 (2021). <https://doi.org/10.1038/s41699-021-00228-x> – **MIT News Feature**

**Lew, A.J.**, Kaser, S.J., Kim, D.Y., Christoff-Tempesta, T., Cho, Y., Ortony, J.H. Effects of molecular flexibility and head group repulsion on aramid amphiphile self-assembly. *Molecular Systems Design & Engineering*. 6, 1016-1024 (2021).

<https://doi.org/10.1039/D1ME00120E>

Christoff-Tempesta, T., Cho, Y., Kim, D.Y., Geri, M., Guillaume, L., **Lew, A.J.**, Zuo, X., Lindemann, W.R., Ortony, J.H. Self-assembly of aramid amphiphiles into ultra-stable nanoribbons and aligned nanoribbon threads. *Nature Nanotechnology*. 16, 447–454 (2021). <https://doi.org/10.1038/s41565-020-00840-w> – Patent Application

**Lew, A.J.**, Christoff-Tempesta, T., Ortony, J.H. Beyond covalent crosslinks: Applications of supramolecular gels. *Gels*. 4, 40 (2018).

<https://doi.org/10.3390/gels4020040>

## Patents -----

**Lew, A.J.**, Buehler, M.J. A Method to Extract Physical Behavior Directly from Simple Visual Empirical Observation Via a Deep Learning Model. U.S. Provisional Patent Application No. 63/333493. Filed April 21, 2022.

Ortony, J., Jia, T., Kim, D. Y., Lindemann, W., Christoff-Tempesta, T., **Lew, A.J.**, & Cho, Y. Aramid amphiphile self-assembled nanostructures. U.S. Patent Application No. 16/825724. Filed September 24, 2020.

## Industry Experience -----

**Spectral Sciences, Inc. – Senior Scientist, Researcher - Scientific Computation** Jan 2024 – Present

- Principal Investigator of Large Language Model project for summarizing and surfacing relationships within scientific content
- Lead research of physics-informed ML models for satellite imagery analysis, supporting AFRL Space Vehicles Directorate
- Software development for AI-enhanced computational fluid dynamics program

**C3 AI – Senior Director, Strategic Solutions** Jan 2023 – Dec 2023

- Created strategic alignment within Fortune 500 clients from users to C-suite on priority AI-addressable problems
- Scoped enterprise-level AI solutions and application roadmaps, generating \$100,000's of value
- Coordinated internal solutions, sales, alliances, strategy, and legal teams to serve client digital transformation

**Boston Consulting Group – Bridge to BCG Program Member** Mar 2022 – Apr 2022

- Strategized while solving a case in a realistic BCG case team simulation
- Teamed with Bridge participants and consultants to understand the why and how behind case work
- Networked with BCG consulting staff and advanced to final round interviews

**Patagonia – Case Competition Consultant** Jan 2020 – Jul 2020

- Collaborated in multidisciplinary team of 6 engineering, business, and science students to reduce Patagonia's textile waste
- Developed and presented solution to a worldwide audience of Patagonia staff, C-suite, and invited guests
- Won 1st place of 130+ teams, awarded \$15,000 and discussions with Patagonia for plans on implementing our solution

**Northrop Grumman – Technical Engineer Intern** Jun 2016 – Sep 2016

- Supported government DARPA "DAHI" program, "NGnext" nanoparticle research, and polymer coating R&D
- Stewarded newly obtained Laser Scanning Confocal Microscope – tool setup, vendor point of contact, trained other engineers
- Attained interim Department of Defense Secret-level Security Clearance for trusted projects

**Northrop Grumman – Process Integration Intern** Jun 2015 – Sep 2015

- Created Excel VBA tools for metric tracking and process flow management
- Investigated correlations between physical properties, processing conditions, and final yields of semiconductor boules
- Evaluated and streamline inspection steps for better process flow

**Northrop Grumman – Process Engineer Intern** Jun 2014 – Sep 2014

- Led optimization study for development of new GaN dicing processes
- Qualified new automatic tools for more efficient InP dicing processes, saving \$50,000/year
- Identified and analyzed defects for hundreds of semiconductor chips

## Leadership Experience -----

### **MIT Civil & Environmental Engineering GradCom – Graduate Student Leader**

Jan 2022 – Dec 2022

- Organized department-wide events to reforge student culture after pandemic isolation
- Informed and welcomed newly admitted students at department open houses
- Hosted town halls to gauge student sentiment of the graduate program

### **Ashdown House Executive Committee – Internal Affairs Chair**

Mar 2020 – May 2021

- Support monthly brunch for the graduate community, cooking 100s of pancakes and waffles.
- Advocate student concerns for COVID-era dorm policies
- Pioneer and organize virtual events to maintain community in a changed world

### **MIT ChemREFS – Confidential Peer Mentor**

Mar 2019 – Dec 2022

- Mediated confidential 1-on-1 meetings with students on interpersonal conflicts and graduate school stresses
- Advocated for chemistry graduate students through survey-based annual Department Chair meetings
- Outreach to local high schools to present chemistry demos and inspire students to pursue STEM

### **MIT Chemistry Department – Teaching Assistant**

Aug 2017 – Dec 2018

- Taught 2 hour-long sections and held 2+ sessions of office hours per week for Course 5.111: Principles of Chemical Science
- Created homework questions, maintained code for online "MITx" portion of the class, tech support for in-person lectures
- Administrative grading and solution key write-up for Course 5.73: Intro to Quantum Mechanics I

### **Materials Research Society @ UCLA – President**

May 2016 – Jun 2017

- Led student board of 14 to restructure MRS@UCLA as a consistently active, officially registered student organization
- Organized events including professional workshops, industry info sessions, and mixers between grad/undergrad students
- Collated student feedback on program in department-wide Town Hall meeting, and advocated results to Department Head

### **SAMPE Bridge Competition Team – Co-Founder, Team Lead, and Mentor**

Dec 2015 – May 2017

- Restarted UCLA involvement in SAMPE competition with a team of 4 others, petitioned department for lab space and resources
- Led student teams in the design, fabrication, and 3-pt bend testing of glass fiber composite beams
- Developed and taught composite processing workshops to facilitate wider participation in SAMPE Bridge Competition.

### **Tau Beta Pi, Epsilon Chapter – Distinguished Member, Officer**

Jun 2015 - Jun 2017

- Taught review sessions for midterm and final exams in general STEM classes
- Held weekly tutoring hours for students across the school of engineering
- Organized joint social events across engineering majors

## Presentations -----

Lew, A.J. Talk: "Accelerating Materials Recipe Acquisition via LLM-Mediated Reinforcement Learning". *MRS Fall Meeting and Exhibit*, Boston (2024)

Lew, A.J. "Elucidating Structure-Property Relationships for Targeted Materials Mechanical Design". *MIT Public Thesis Defense*, Cambridge (2022)

Lew, A.J., Buehler, M.J. Talk #2011619: "Leveraging Deep Learning Models to Expedite and Expand the Exploration of Material Structures for Mechanical Design". *10th International Conference on Multiscale Materials Modeling*, Baltimore (2022)

Lew, A.J., Gilbert, P.U.P.A., Buehler, M.J. Poster #SF12.11.06: "Non-destructive Hardness Prediction via Deep Learning Image Regression Models". *MRS Spring Meeting and Exhibit*, Virtual (2022) – **Outstanding Contribution**

Lew, A.J., Buehler, M.J. Talk #DS03.03.04: "A Deep Learning Augmented Genetic Algorithm Approach for 2D Fracture Discovery and Design". *MRS Fall Meeting and Exhibit*, Boston (2021)

Lew, A.J., Buehler, M.J. Talk: "Cutting Through Failure by Traversing Across Disciplines: Leveraging Traditional Mechanics, Deep Learning, and Genetic Algorithms to Predict Fracture and Design Material Structure". *MIT Chemistry Student Seminar*, Cambridge (2021)

Lew, A.J., Buehler, M.J. Talk #21721056: "Using Deep Learning to Predict Fracture: Analysis, Design, and Additive Manufacturing". *16th US National Congress on Computational Mechanics*, Virtual (2021) – **Keynote Address**

Lew, A.J., Kim, DY, Ortony, J.H. Poster: "From Molecules to Macroscale: Self-assembly of Robust Hierarchically Ordered Materials". *MIT WIC/CADI Poster Symposium*, Cambridge (2019)

Lew, A.J., Machness, A., Goorsky, M. Poster #557: "Synthesis and Characterization of Superparamagnetic Iron Oxide Nanoparticles for Magnetic Hyperthermia Applications". *UCLA Undergraduate Research Week*, Los Angeles (2017) – **Vice Provost's Poster Recognition Award**

Lew, A.J., Lieng, J., Tran, V., Wolfman, J. Poster Category D: "I Beam Glass Fiber". SAMPE Conference and Exhibition, Seattle (2017)

Lang, A., Cruz, A., Reyes, A., Lew, A.J., Sulian, A., Lara, A., Del Signore, C., Kotcherha, C., Webber, D., Babiker, H., Wu, J., Cho, K., Matsui, K., Johnson, L., Conde, L., Gutierrez, N., Saepoo, S., Slavin, S., Akiyama, T. Poster: "Microelectronics: Micro-design, Mega-impact". *Northrop Grumman Intern Showcase: Explore Space*, Redondo Beach (2016) – **Best Overall Presentation Award**

Lew, A.J., Timmons, J., Lieng, J., Figueroa, J., Chu, K. Poster Category E: "Square Beam Glass Fiber", *SAMPE Conference and Exhibition*, Long Beach (2016)

Lew, A.J., Machness, A., Goorsky, M. Poster #42: "Synthesis and Characterization of Superparamagnetic Iron Oxide Nanoparticles with Varying Precursor Addition Rate". *ACS Southern California Undergraduate Research Conference*, Long Beach (2016) – **Outstanding Poster Award**

Skills -----

#### **Computational Modeling**

- *General* – Python (LangChain, PyTorch, TensorFlow, Keras, Scikit-Learn, NumPy, Matplotlib, Pandas, Jupyter), RDKit, HTML, Bash
- *Classical Simulation* – Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), Open Visualization Tool (OVITO)
- *Artificial Intelligence* – Large Language Models, Transformer Models, Diffusion Models, Graph Neural Network, Convolutional Neural Network, Residual Neural Network, Long Short-Term Memory Network, Variational Autoencoder, Genetic Algorithm, Bayesian Optimization, Reinforcement Learning, Supervised Learning, Unsupervised Learning

#### **Laboratory Techniques**

- *Organic Synthesis* – Peptide Coupling, BOC-protection/deprotection, Column Chromatography
- *Characterization* – Nuclear Magnetic Resonance ( $^1\text{H}$ NMR &  $^{13}\text{C}$ NMR), Thin Layer Chromatography (TLC), Mass Spectrometry (MS), UV-Visible Spectrophotometry (UV-Vis), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), X-Ray Diffraction (XRD), Förster Resonance Energy Transfer (FRET), Compression Testing

#### **Interpersonal Qualifications**

- *Mentorship* – Classroom Teaching, 1-on-1 Tutoring, Hands-on Workshops, Teaching Assistant
- *Business* – Miller Heiman Strategic and Conceptual Sales Certification, C3 AI Application Development Methodology Certification
- *Discretion* – Department of Defense Secret-level Security Clearance, Confidential Conflict Mediation Training Certification