Channyung Lee

(+1)217-419-1821 | cl104@illinois.edu | https://scholar.google.com/citations?user=mW8w0G0AAAAJ
| channyung-lee-8269b0201 | 104 S. Goodwin Ave. M/C 230, Urbana, IL, 61801

Professional Summary

Materials scientist specializing in quantum computational chemistry and machine learning applications for fundamental science problems. Experienced in developing first-principles simulation frameworks to investigate transport mechanisms, electronic structures, and phase transformations across diverse material systems. Skilled in integrating density functional theory with machine learning approaches to accelerate materials discovery and understand complex reaction processes.

Quantum Computational Chemistry: Density Functional Theory (VASP, Quantum ESPRESSO) | Electronic Structure Calculations | Optical Calculations | Reaction Pathway Analysis | Temperature-dependent Properties

Machine Learning for Chemistry: Surrogate Models for Alloy Energy Predictions | Interatomic Potentials Development | Monte Carlo Methods | Data Analysis & Statistical Modeling | Open Source Tool Development (KROGER)[Link]

Computational Modeling: First-principles Simulations | Master Diffusion Equations | Defect Thermodynamics | Phase Transformation Modeling | Multi-scale Simulation Approaches

Programming & Development: Python | C | Matlab | R | High-performance Computing | Algorithm Development

Education & Internship

University of Illinois Urbana-Champaign (UIUC) *Urbana, IL, USA*
Ph.D. candidate in Mechanical Science and Engineering (GPA: 3.95/4.00, Prof. Elif Ertekin) Jan. 2021 - Present

Seoul National University (SNU) *Seoul, Rep. of Korea*
MS in Mechanical Engineering (GPA: 4.00/4.00, Prof. Mansoo Choi) Mar. 2018 - Feb. 2020

Seoul National University (SNU) *Seoul, Rep. of Korea*
BS in Mechanical and Aerospace Engineering (GPA: 3.72/4.00) Mar. 2012 - Feb. 2018

Lawrence Livermore National Laboratory (LLNL) *Livermore, CA, USA*
Internship at Quantum Simulations Group (Dr. Joel B. Varley) Jun. 2023 - Aug. 2023

Korea Institute of Science and Technology (KIST) *Seoul, Rep. of Korea*
Internship at Center for Energy Materials Research (Prof. Hyoungchul Kim) Jan. 2020 - Dec. 2020

Technical Skills

Programming	Python, C, Matlab, R, LaTeX
Simulation	Density Functional Theory (VASP, Quantum ESPRESSO), Monte Carlo, Machine Learning for Materials Science
CAD & FEM	Solidworks, CATIA, Abaqus
Analysis Tools	SEM, AFM, XRD, Photolithography, Impedance Spectroscopy (EIS)

Research Projects

Global Frontier R&D Program on Center for Multiscale Energy Systems *Seoul, Rep. of Korea*
The Ministry of Science and ICT, Republic of Korea (Grant No. 2012M3A6A7054855) Jan. 2018 - Dec. 2020

- Developed novel micro-patterning techniques using soft-lithography to enhance electrode-electrolyte interfaces in solid oxide fuel cells (SOFCs)
- Created data analysis tools for advanced electrochemical impedance spectroscopy (EIS) with distribution of relaxation times (DRT) to precisely characterize interfacial processes in energy conversion devices

Computational Modeling of Defect Equilibria in β-Ga_2O_3 *Urbana, IL, USA*
The Air Force Office of Scientific Research (Award No. FA9550-21-0078) Jun. 2021 - Dec. 2024

- Created breakthrough approaches for commercialization through advanced defect engineering, providing unprecedented control over electronic properties in power devices
- Developed comprehensive computational frameworks and MATLAB tools (KROGER) for quantitative modeling of defect concentrations in wide bandgap semiconductors, enabling precise prediction of electronic properties under various growth conditions

MURI: β-Ga_2O_3 as a High-Critical Field Strength Material for Power Systems *Urbana, IL, USA*

The Air Force Office of Scientific Research (Award No. FA9550-21-0078) Jun. 2021 - Dec. 2024

- Investigated defect diffusion mechanisms in β-Ga_2O_3 using first-principles calculations and master diffusion equations
- Established optimal doping strategies by determining formation energies and diffusion characteristics of acceptors and donors using first-principles calculations

Advanced Alloy Design: Defect Engineering in Complex Systems (2023 IRG2) *Urbana, IL, USA*

Illinois Materials Research Science and Engineering Center (I-MRSEC) (NSF Award No. DMR-2309037) Jun. 2023 - Present

- Led computational alloy design research focusing on energy prediction and defect thermodynamics in multi-component systems including high entropy alloys and disordered oxides
- Developed first-principles frameworks to predict formation energies and defect equilibria in complex alloy systems, enabling rational design of materials with tailored transport and mechanical properties
- Established quantitative structure-property relationships linking alloy composition, defect concentration, and macroscopic properties through integrated computational approaches

Publications

[1] **Channyung Lee**, Sung Soo Shin, Jiwoo Choi, Jinhyeon Kim, Ji-Won Son, Mansoo Choi*, and Hyun Ho Shin*, "A micro-patterned electrode/electrolyte interface fabricated by soft-lithography for facile oxygen reduction in solid oxide fuel cells", *J. Mater. Chem. A*(2020) [Link]

[2] **Channyung Lee**≈, Sung Soo Shin≈, Jinhyeon Kim, Jiwoo Choi, Mansoo Choi*, and Hyun Ho Shin*, "Tailoring an Interface Microstructure for High-Performance Reversible Protonic Ceramic Electrochemical Cells via Soft Lithography", *ACS Appl. Mater. Interfaces*(2022) [Link](≈ equal contribution)

[3] **Channyung Lee**, Nathan D. Rock, Ariful Islam, Michael A. Scarpulla, and Elif Ertekin*, "Electron-phonon effects and temperature-dependence of the electronic structure of monoclinic β-Ga_2O_3", *APL Mater.*(2023)[Link]

[4] Hyeseong Jeong, **Channyung Lee**, Ji-Won Son, Seung Yong Lee, Kyung Joong Yoon, Dong Wook Shin, Mansoo Choi, Sung Soo Shin*, and Hyoungchul Kim*, "Advancing towards ready-to-use solid oxide fuel cells: 5-minute start-up with 1.1 W power at 600 °C", *J. Mater. Chem. A* (2023)[Link]

[5] **Channyung Lee**, Michael A Scarpulla, and Elif Ertekin*, "Investigation of Ga interstitial and vacancy diffusion in β-Ga_2O_3 via split defects: A direct approach via master diffusion equations", *Phys. Rev. Mater.* (2024)[Link][Link]

[6] Emily J Skiba≈, Haley B Buckner≈, **Channyung Lee**≈, Grace McKnight≈, Rachel F Wallick, Renske van der Veen, Elif Ertekin, and Nicola H Perry*, "UV-Driven Oxygen Surface Exchange and Stoichiometry Changes in a Thin-Film, Nondilute Mixed Ionic Electronic Conductor, Sr(Ti,Fe)O_{3-d}", *J. Am. Chem. Soc.* (2024)[Link] (≈ equal contribution)

[7] Andrew R Balog*, **Channyung Lee**, Daniel Duarte-Ruiz, Sai Venkata Gayathri Ayyagari, Jani Jesenovec, Adrian E Chmielewski, Leixin Miao, Benjamin L Dutton, John McCloy, Caterina Cocchi, Elif Ertekin, and Nasim Alem*, "Determination of the β to γ Phase Transformation Mechanism in Sc- and Al-Alloyed β-Ga_2O_3 Crystals", *Appl. Electron. Mater.* (2024)[Link]

[8] **Channyung Lee**, Michael A Scarpulla, Joel B. Varley, and Elif Ertekin*, "Unraveling the transformation pathway of the β to γ phase transition in Ga_2O_3 from atomistic simulations", *Phys. Rev. Mater.* (2025)[Link]

[9] Khandakar Aaditta Arnab, Megan Stephens Isaac Maxfield, **Channyung Lee**, Elif Ertekin, Ymir Frodason, Joel B Varley, Mike Scarpulla*, "Quantitative Modeling of Point Defects in β-Ga_2O_3 Combining Hybrid Functional Energetics with Semiconductor and Processes Thermodynamics", *Phys. Chem. Chem. Phys., Accepted* (2025)[Link]

[10] A K M Ashiquzzaman Shawon, Ferdaushi Bipasha; **Channyung Lee**, Kamil Ciesielski, Brian Tijan, Eric Toberer, Elif Ertekin, and Alexandra Zevalkink, "Ag vacancies as 'killer-defects' in CaAgSb thermoelectrics", *ACS Appl. Energy Mater.*(2025)[Link]

[11] Grace McKnight≈, **Channyung Lee**≈, and Elif Ertekin*, "Investigation of O interstitial diffusion in β-Ga_2O_3 : a direct approach via master diffusion equations", *Phys. Rev. B, accepted* (2025) (≈ equal contribution)[Link]

[12] **Channyung Lee**, Michael A Scarpulla, Elif Ertekin*, and Joel B Varley*, "Diffusion of acceptor dopants in monoclinic β-Ga_2O_3", *Phys. Rev. Mater., in review* (2025)[Link]

[13] Andrew R Balog≈, **Channyung Lee**≈, Elif Ertekin* and Nasim Alem*, "Scandium Occupancy and Extended Defect Formation in Alloyed β-$(Sc_xGa_{1-x})_2O_3$ Single Crystals", *in prep.* (2025) (≈ equal contribution)

[14] **Channyung Lee**≈, Hong-Jyun Huang≈, Nicola H Perry, and Elif Ertekin*, "Magnetic and Structural Ordering in $SrTi_{1-x}Co_xO_{3-\delta}$ Perovskite Alloys", *in prep.* (2025) (≈ equal contribution)

[15] **Channyung Lee**, Hong-Jyun Huang, Amir M. Orvati Movaffagh, Sara Kadkhodaei, Nicola H Perry, and Elif Ertekin*, "Defect Equilibria in $SrTi_{1-x}Fe_xO_{3-\delta}$ Perovskite Alloys", *in prep.* (2025)

Other Experiences

Project Review *Arlington, VA*

Air Force Office of Scientific Research (AFOSR) Review Oral Presentations May 2024

International Academic Conferences *Several Cities*

Oral/Poster Presentations Jan. 2018 - Present

- ACS Fall 2018 National Meeting, Boston, MA, 2018 (Oral)
- The 22nd International Conference on Solid State Ionics, Pyeongchang, Rep. of Korea, 2019 (Poster)
- Defects in Semiconductors - Gordon Research Conferences, New London, NH, USA, 2022 (Poster)
- The 6th US Workshop on Gallium Oxide (GOX 2023), Buffalo, NY, USA, 2023 (Oral)
- International Conference on Defects in Semiconductors (ICDS), Rehoboth Beach, DE, USA, 2023 (Poster)
- Joint March Meeting and April Meeting: Global Physics Summit 2025, Anaheim, CA, USA, 2025 (Oral)

References

- Prof. Elif Ertekin
  Associate Professor, Ph.D., at University of Illinois Urbana-Champaign, Urbana, IL, USA
  ertekin@illinois.edu
- Prof. Michael A. (Mike) Scarpulla
  Associate Professor, Ph.D., at The University of Utah, Salt Lake City, UT, USA
  scarpulla@ece.utah.edu
- Prof. Mansoo Choi
  Professor Emeritus, Ph.D., at Seoul National University, Seoul, South Korea
  mchoi@snu.edu