Curriculum Vitae

Seongjoo Jung

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Education

University of Minnesota — Minneapolis, MN, USA
Ph.D. Candidate, Chemical Engineering (GPA 4.00/4.00) — 2020–present
Department of Chemical Engineering and Material Science (CEMS)
Advisors: Turan Birol, Paul J. Dauenhauer

Seoul National University — Seoul, Korea
Bachelor of Science, Major in Chemical and Biological Engineering — 2015–2020
Minor in Computer Science and Engineering
Honors: summa cum laude
Advisors: Yung-Eun Sung

Research Experiences

Graduate Researcher, University of Minnesota — 2020–present

- Ferroelectric origin of fluorite HfO_2
  - Mapped the energy landscape of entire order parameter space and identified the minimum energy pathway for ferroelectric HfO_2 by symmetry-guided DFT calculations.
  - Identified the novel mechanism for ferroelectricity in HfO_2 which is distinct from any previously considered proper or improper category.
- Octahedral rotation-induced antiferroelectricity in perovskite structure crystals
  - Predicted high polarization-rotation coupling from discontinuous behavior in spontaneous polarization and octahedral rotation for I4cm-P4mm phase transition in perovskites.
  - Demonstrated that the coupling between polarization and non-polar octahedral rotations in perovskites can cause antiferroelectric-like double hysteresis under epitaxial strain.
  - Designed antiferroelectric-like Ruddlesden-Popper phases and superlattice structures with low critical field based on phonon frequencies and rotation-polarization coupling.
- DFT modeling of dynamic catalysis on ferroelectric catalytic capacitors
  - Developed polarized-ground state calculation for VASP (commercial ab initio quantum mechanical calculations software) using Fortran and Python.
  - Analyzed ferroelectric thin-film $Pt/PbTiO_3$ systems at different support polarization geometrically and electronically using Bader, DDEC6 charges, (integrated) PDOS, real-space charge density, demonstrating interface effects on surface active sites.
  - Discovered breaking of transition-state scaling relations using CI-NEB based on adsorption energy changes related to d-band structure changes.

Research Intern, Seoul National University and Korea Center for Artificial Photosynthesis — 2018–2019

Awards and Honors

Kokes Award — 2023

- North American Catalysis Society

The Lanny & Charlotte Schmidt and Duane Goetsch & Nancy M. Dickerson Fellowship 2021

- CEMS, University of Minnesota

Fridley Fellowship 2021

- CEMS, University of Minnesota

Peter and Gene Pierce Fellowship 2021

- CEMS, University of Minnesota

Samsung Convergence Software Course Scholarship 2017–2020

- Samsung Electronics. Minor program with scholarship for selected non-computer science major students

National Scholarship for Science and Engineering (full tuition) 2015–2020

- Ministry of Science and ICT, Korea. Provided full tuition coverage for 48 months

External Research Resources

Discover ACCESS Allocations 2023–2024

- National Science Foundation

ACCESS (formerly XSEDE) Startup Allocations 2022–2023

- National Science Foundation

Teaching and Mentorship

Teaching Assistant, University of Minnesota

- ChEn 3101: Chemical Engineering Thermodynamics Spring 2023
  - Head TA and Recitation TA. Taught 10 sessions of recitation to students, provided office hours and supplementary course materials.
- ChEn 4401W: Senior Chemical Engineering Lab (Unit Ops) Fall 2021
  - Lab TA for distillation, gas membrane separation, non-Newtonian pipe flow, ion exchange, humidification & water-cooling experiments. Grading TA for humidification & water-cooling experiment.

Mentor, Hyeonseo (Harry) Park

- Mentorship on DFT calculations, solid state physics, group theory and research topic: charge density wave phase diagram of dichalcogenide $TiSe_2$

Talks and Conferences

AIChE Annual Meeting, San Diego, CA Oct 2024

"Microscopic Mechanism of Polarization Switching in Ferroelectric HfO_2"

"Rotation-Induced Double Hysteresis of Perovskites for Energy Storage"

"Computational Modelling of Dynamic Charge and Adsorption Responses"

IEEE Ultrasonics, Ferroelectrics, and Frequency Control Joint Symposium, Taipei, Taiwan Sep 2024

"Rotation Induced Antiferroelectric-Like Double Hysteresis of $SrTiO_3$ and $BaZrO_3$"

American Physical Society March Meeting, Minneapolis, MN Mar 2024

"Rotation Induced Antiferroelectric-like Double Hysteresis of Perovskites"

North American Catalysis Society Meeting, Providence, RI Jun 2023

"Support Polarization Control of Catalysts: Elucidating and Breaking Scaling Relations"

Gordon Conference – Catalysis, New London, NH (Accepted) Jun 2022

"Catalyst Charge Injection via Polarized Ferroelectric Support-Metal Interaction"

Programming Skills

Python; MATLAB; Java; Unix; LaTeX; HTML/CSS; JavaScript; Git; PyTorch; C; C++; FORTRAN;

Publications

Jung S., Pizzolitto C., Biasi P., Dauenhauer P. J., Birol, T. "Programmable Catalysis by Support Polarization: Elucidating and Breaking Scaling Relations", *Nature Communications* **14**, 7795 (2023)

Jung S., Birol, T. "Rotation-Induced, Antiferroelectric-like Double Hysteresis in $SrTiO_3$" (To be submitted, manuscript available upon request)

Gathmann S. R., **Jung S.**, Frisbie D., Dauenhauer P. J. "Catalytic Resonance Theory: Parametric Uncertainty on Microkinetic Predictions of Dynamic Rate Enhancement" (To be submitted)

Jung S., Birol, T. "Novel mechanism of ferroelectricity in HfO_2" (To be submitted)

Park H., **Jung S.**, Birol, T. "Group Theoretical Analysis of Charge Density Wave Transition and Chirality in 1T-$TiSe_2$" (In Progress)