#### 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

Minor in Computer Science and Engineering

Honors: summa cum laude Advisors: Yung-Eun Sung 2015–2020

### Research Experiences

#### Graduate Researcher, University of Minnesota

 $2020{\rm -present}$ 

- Ferroelectric origin of fluorite HfO<sub>2</sub> (Work in progress)
  - Identified microscopic mechanisms of single-domain phase transition from tetragonal to ferroelectric  $HfO_2$  and its polarization switching.
- Octahedral rotation-induced antiferroelectricity in perovskite structure crystals
  - Constructed Landau free energy expression of perovskite structures with space group I4cm, using polarization and octahedral rotation as order parameters.
  - Identified minimum electric enthalpy pathway of polarization switching and discovered antiferroelectric hysteresis at the interface of I4cm-P4mm phase.
  - Designed antiferroelectric Ruddlesden-Popper phases and superlattice structures based on phonon frequencies and rotation-polarization coupling.
- DFT modelling 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<sub>3</sub> 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.
  - Predicted adsorption energy changes related to d-band structure changes, and discovered breaking of transition-state scaling relations using CI-NEB.

Research Intern, Seoul National University and Korea Center for Artificial Photosynthesis

2018 – 2019

### **Awards and Honors**

Kokes Award 2023

• North American Catalysis Society

• CEMS, University of Minnesota

Fridley Fellowship 2021

• CEMS, University of Minnesota

Peter and Gene Pierce Fellowship

• CEMS, University of Minnesota

Samsung Convergence Software Course Scholarship

2017-2020

2021

• 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<sub>2</sub>

### Talks and Conferences

AIChE Annual Meeting, San Diego, CA

Oct 2024

"Microscopic Mechanism of Polarization Switching in Ferroelectric HfO<sub>2</sub>"

"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<sub>3</sub> and BaZrO<sub>3</sub>"

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"

"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**

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

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

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

**Jung S.**, Birol, T. "Origin of ferroelectricity in flourite HfO<sub>2</sub>" (In Progress)