

## Eunseok Lee

Mechanical and Aerospace Engineering  
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### EDUCATION

**Ph.D. in Mechanical Engineering with minor in Physics, Stanford University, Jan 2011**

- Depth area: Mechanics and Computation Division
- Dissertation: Kinetic Monte Carlo Model of the Ionic Conduction in Bulk Yttria-stabilized Zirconia

**M.S. in Mechanical Engineering, Stanford University, Aug 2005**

**B.S. in Mechanical Engineering, Seoul National University, Feb 2001**

### PROFESSIONAL APPOINTMENTS

**University of Alabama in Huntsville, Huntsville, AL, Aug 2014–present**

Assistant Professor, Mechanical and Aerospace Engineering

**Lawrence Berkeley National Laboratory, Berkeley, CA, Jan 2011–Jul 2014**

Postdoctoral Fellow, Environmental Energy Technologies Division

**Computational Modeling Consultants, Inc., Wellesley, MA, Jun 2013–Jul 2014**

Senior Researcher

### RESEARCH INTERESTS

- Atomistic and multiscale computational methods
- Data-driven science; a materials genome approach
- Electrochemical energy conversion/storage systems
- Micro- and nano-mechanics, kinetics, and transport

### RESEARCH EXPERIENCE

**Assistant Professor, University of Alabama in Huntsville, Aug 2014–present**

- Understanding the effects of dopants in transition-metal oxides, for Li-ion batteries
- Mechanical strain effect on the ionic conductivity of solid electrolytes
- Molecular dynamics simulation approach for dynamics fragmentation

**Postdoctoral Fellow, Lawrence Berkeley National Laboratory, 2011–Jul 2014**

- Studied the physical and chemical behaviors in the electrode materials (spinel, graphene, composite materials) of Li-ion batteries, using high-throughput *ab initio* computations, as a part of the DOE's *Batteries for Advanced Transportation Technologies* program.
- Collaborated with several experimental research groups in the lab, *GM*, and *Envia Systems*.

**Senior Researcher, Computational Modeling Consultants, Inc., 2013–Jul 2014**

- Served as a modeling consultant for *P&G* for their development of a new primary battery.

**Research Assistant, Stanford University, 2004–2010**

- Studied the ionic conduction in yttria-stabilized zirconia, a popular solid electrolyte material of the solid electrolyte fuel cell, and suggested a design principle to improve the conductivity, as a part of the DOE's *Energy Frontier Research Center* program at Stanford University.
- Developed a new impedance calculation method using the fluctuation-dissipation theorem.

- Contributed to a new method to calculate the electromagnetic structure of materials, as a part of Quantum Simulations of Materials and Nanostructures project of the DOE's *SciDAC* program.

### **Summer Student Scholar in Computational Chemistry and Material Science Summer Institute, Lawrence Livermore National Laboratory, Jun–Aug 2005**

- Participated in the project for developing a new method to calculate the energy of system under a magnetic field and implementing it in a density functional theory computational code.

## **PUBLICATIONS**

### **Refereed Journal Publications**

- Jung-Hyun Kim, Ashfia Huq, Miaofang Chi, Nicholas P.W. Pieczonka, Eunseok Lee, Misle Tessema, Craig A. Bridges, Arumugam Manthiram, Kristin A. Persson, Bob R. Powell, "Integrated Nano-Domains of Disordered and Ordered Spinel Phases in  $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$  for Li-Ion Batteries", *Chemistry of Materials* **26**, 4377-4386 (2014).
- Eunseok Lee and Kristin Persson, "Structural and Chemical Evolution of the Layered Li-excess  $\text{Li}_x\text{MnO}_3$  as a function of Li content from First-Principles Calculations", *Advanced Energy Materials* **4**, 1400498 (2014).
- Eunseok Lee and Kristin Persson, "First-principles study of the nano-scaling effect on the electrochemical behavior in  $\text{Li}_x\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ ", *Nanotechnology* **24**, 424007 (2013).
- Eunseok Lee and Kristin Persson, "Solid-Solution Li Intercalation as a Function of Cation Order/Disorder in the High-Voltage  $\text{Li}_x\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$  Spinel", *Chemistry of Materials* **25**, 2885 (2013).
- Eunseok Lee and Kristin Persson, "Li Absorption and Intercalation in Single Layer Graphene and Few Layer Graphene by First Principles", *Nano Letters* **12**, 4624 (2012).
- Eunseok Lee and Kristin Persson, "Revealing the coupled cation interactions behind the electrochemical profile of  $\text{Li}_x\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ ", *Energy & Environmental Science* **5**, 6047-6051 (2012).
- Eunseok Lee, Friedrich B. Prinz, and Wei Cai, "Ab initio kinetic Monte Carlo model of ionic conduction in bulk Yttria-stabilized zirconia", *Modeling Simul. Mater. Sci. Eng.* **20**, 065006 (2012).
- Eunseok Lee, Friedrich B. Prinz, and Wei Cai, "Enhancing Ionic Conductivity of Bulk Single Crystal Yttria-stabilized Zirconia by Tailoring Dopant Distribution", *Physical Review B* **83**, 052301 (2011).
- Eunseok Lee, Friedrich B. Prinz, and Wei Cai, "Kinetic Monte Carlo simulations of oxygen vacancy diffusion in a solid electrolyte: Computing the electrical impedance using the fluctuation-dissipation theorem", *Electrochemistry Communications* **12**, 223 (2010).
- Eunseok Lee, Wei Cai, and Giulia Galli, "Electronic structure calculations in a uniform magnetic field using periodic supercells", *Journal of Computational Physics* **226**, 1310 (2007).

## **CONFERENCE EXPERIENCE**

### **Session Chair**

- International Mechanical Engineering Congress & Exposition (IMECE) 2015 - Track 7-9-7: Electrochemical Energy Conversion and Storage 3, Houston, TX, Nov 2015.
- Material Research Society Spring Meeting - Session F18: Graphene, San Francisco, CA, Apr 2013.

### **Oral Presentation**

- Eunseok Lee, "First-principles Study on the Interface Between  $\text{Li}_4\text{PO}_3\text{N}-\text{BaTiO}_3$  and Ni-Mn Spinel", International Mechanical Engineering Congress & Exposition (IMECE) 2015, Houston, TX, Nov 2015.

- Eunseok Lee, “Ab-initio-based Cluster Expansion Study of the Phase Transformation and Voltage Fade of the Layered  $\text{Li}_x\text{MnO}_3$ ”, 7<sup>th</sup> International Conference on Multiscale Materials Modeling, Berkeley, CA, Oct 2014.
- Eunseok Lee and Kristin Persson, “First-Principles Calculations Study on the Electrochemical Activity and Structural Stability of the  $\text{Li}_2\text{MnO}_3$ ”, 224<sup>th</sup> Electrochemical Society meeting, San Francisco, CA, Oct 2013.
- Eunseok Lee and Kristin Persson, “First-Principles Study of the Nano-scaling Effect on the Rate Capability in  $\text{Li}_x\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ ”, 224<sup>th</sup> Electrochemical Society meeting, San Francisco, CA, Oct 2013.
- Eunseok Lee and Kristin Persson, “Coupling between Cation Interaction and Electrode Performance in High Voltage  $\text{Li}_x\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ ”, Material Research Society 2013 Spring Meeting, San Francisco, CA, Apr 2013.
- Eunseok Lee and Kristin Persson, “Li absorption in Single Layer Graphene, Few layer Graphene, and Bulk Graphite”, Material Research Society 2013 Spring Meeting, San Francisco, CA, Apr 2013.
- Eunseok Lee and Kristin Persson, “First-Principles Study of the Ionic Ordering in  $\text{Li}_x\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ ”, 221<sup>st</sup> Electrochemical Society meeting, Seattle, WA, May 2012.
- Eunseok Lee and Kristin Persson, “First-Principles Study of Li Absorption in Single Layer Graphene, Few Layer Graphenes, and Bulk Graphite”, 221<sup>st</sup> Electrochemical Society meeting, Seattle, WA, May 2012.
- Kristin Persson and Eunseok Lee, “Origin of the Voltage Profile in Ordered/Disordered  $\text{Li}_x(\text{Ni}_{0.5}\text{Mn}_{1.5})\text{O}_4$ ”, Material Research Society 2012 Spring Meeting, San Francisco, CA, Apr 2012.
- Eunseok Lee, Friedrich B. Prinz, and Wei Cai, “Kinetic Monte Carlo model of ionic conductivity in YSZ”, Material Research Society 2009 Fall Meeting, Boston, MA, Dec 2009.
- Eunseok Lee, Friedrich B. Prinz, and Wei Cai, “Computing electrochemical Impedance of Solid Electrolyte from fluctuations”, Material Research Society 2008 Fall Meeting, Boston, MA, Dec 2008.
- Eunseok Lee, Friedrich B. Prinz, and Wei Cai, “Computing electrochemical Impedance of Solid Electrolyte from fluctuations”, 4<sup>th</sup> International Conference on Multiscale Materials Modeling, Tallahassee, FL, Oct 2008.
- Eunseok Lee, Friedrich B. Prinz, and Wei Cai, “Computing electrochemical Impedance of Solid Electrolyte from fluctuations”, 214<sup>th</sup> Electrochemical Society meeting, Honolulu, HI, Oct 2008.

#### **Poster Presentation**

- Eunseok Lee, Friedrich B. Prinz, and Wei Cai, “Computing electrochemical Impedance of Solid Electrolyte using the fluctuation-dissipation theorem”, Material Research Society 2007 Fall Meeting, Boston, MA, Nov 2007.
- Eunseok Lee, Wei Cai, and Giulia Galli, “Ab initio Calculation in Uniform Magnetic Field Using Periodic Supercell”, Berkeley Nanoforum 2005, Berkeley, CA, Apr 2005.

#### **PROFESSIONAL PRESENTATION**

##### **“First-Principles Research on Materials for Li-ion Batteries”**

- CFD Research Corporation, 6/19/15

##### **“Understanding the Phase Transformation Mechanism of $\text{Li}_2\text{MnO}_3$ from First-principles”**

- Seoul National University, Mechanical and Aerospace Engineering, 5/12/15
- Yonsei University, Mechanical Engineering, 5/26/15
- University of Illinois at Chicago, Chemistry, 12/8/14
- Northwestern University, Materials Science and Engineering, 12/5/14
- Argonne National Laboratory, Chemical Science and Engineering, 12/4/14
- Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, 11/24/14

**“First-Principles Calculations Study on the Electrochemical Activity and Structural Stability of the  $\text{Li}_2\text{MnO}_3$ ”**

- Lawrence Berkeley National Laboratory, BATT seminar, 5/24/14

**“Atomistic Description of the Electrochemical Behaviors in the Li-ion Battery Electrode Materials”**

- Ulsan National Institute of Science & Technology, Energy and Chemical Engineering, 6/7/13
- Kyungpook National University, Mechanical Engineering, 6/5/13
- Pohang University of Science and Technology, Materials Science and Engineering, 6/4/13
- Yonsei University, Mechanical Engineering, 5/29/13
- Samsung SDI, Corporate R&D Center, 5/27/13
- Daegu Gyeongbuk Institute of Science & Technology, Energy Systems Engineering, 5/21/13
- Korea Advanced Institute of Science & Technology, Materials Science and Engineering, 5/20/13
- Seoul National University, Materials Science and Engineering, 5/13/13

**TEACHING EXPERIENCE****Instructor, Mechanical and Aerospace Engineering, University of Alabama in Huntsville**

- MAE 671: Continuum Mechanics (Spring 2016)
- MAE 695ST: Computational Nanotechnology (Fall 2015)
- MAE 778: Fracture Mechanics (Fall 2015)
- MAE 574: Applied Mechanics of Solids (Spring 2015, Spring 2016)
- MAE/CE 672: Elasticity (Fall 2014)

**Teaching Assistant, Mechanical Engineering Department, Stanford University**

- ME 340A: Theory and Application of Elasticity (2005, 2006)
- ME 340B: Elasticity in Microscopic Structures (2005)
- ME 334: Introduction to Statistical Mechanics (2006, 2007)
- ME 346: Molecular Simulations (2004)

**AWARDS AND HONORS**

- New Faculty Research award (2015) – University of Alabama in Huntsville
- Samsung Scholarship for studying abroad (2005-2009) – Samsung LeeGunHee Scholarship Foundation (currently, Samsung Scholarship Foundation)

**AUXILIARY INFORMATION**

Mandatory military requirement in Republic of Korea Army, 2001–2003