Donghee Chang, PhD

Materials Science research Scientist/Engineer

Greensboro, NC. USA • (949)408-5872 • doch@umich.edu • Google Scholar Link

EDUCATION

PhD in Materials Science & Engineering, University of Michigan, Ann Arbor May 2015
Thesis title: "Elucidating the origins of hysteresis and reaction mechanisms of electrode materials for Li and Na batteries"

BS in Chemical Engineering / Materials Science, University of California, Davis May 2010

PROFESSIONAL EXPERIENCE

R&D Team lead, Soelect INC., NC, USA Oct. 2023-Present

- Lead R&D projects:
  - Conducted extensive literature reviews to identify opportunities for innovation in battery technology.
  - Designed and executed hands-on experiments for developing new products like Li-S batteries and Li metal anodes for high-salt concentration electrolytes.
  - Conducted performance evolutions and data analysis to assess cell performance and identify improvement areas.
- Developed electrochemical analysis systems:
  - Designed and implemented Python-based electrochemical analysis systems (Dash, pandas, plotly) for data collection and analysis.
  - Established a web-based cell data plotting platform to gain insights into overall battery performance, facilitating informed decision-making in R&D projects.
- Participated in DOE proposals:
  - Collaborated with cross-functional teams to develop proposals submitted to the Department of Energy (DOE), securing funding for R&D initiatives in the technology sector.
- Created teaching materials for the Guilford Technical Community College (GTCC) Battery Certification Training Program:
  - Developed educational materials and curriculum content to enhance student learning and understanding of battery technology concepts.
- Prepared technical support for patents:
  - Provided technical support for patent applications, including conducting patent searches and preparing documentation to support patent filings.

Senior Cell Engineer, Xos INC., CA, USA March. 2022-April.2023

Computational Techniques: Python (pandas, Dash)
Characterization Techniques: XRD, TGA, SEM-FIB, Rheometer, and Karl Fisher Titration

- Led the development of Li-S battery chemistry:
  - Focused on developing practical energy density Li-S battery cells suitable for high-duty electric trucks.
- Tested and analyzed cell cycle performance:

    - Conducted comprehensive testing and analysis of cell cycle performance to identify root causes of cell failure and enable further optimization efforts.
- Developed web-based dashboard for cell cycle data analysis:
    - Designed and implemented a user-friendly web-based dashboard for analyzing cell cycle data, enhancing data visualization and decision-making processes.
- Performed electrode material characterization:
    - Utilized characterization techniques including SEM, TGA, and XRD to analyze and characterize electrode materials, providing critical insights into material properties and performance.
- Prepared technical reports for strategic decision-making:
    - Compiled and presented technical reports summarizing research findings, and test results to internal stakeholders, informing strategic decision-making processes and project directions.
- Established and maintained lab testing facilities:
    - Successfully set up and maintained laboratory testing facilities, ensuring equipment functionality and availability to support ongoing research and development activities.

Senior researcher, LG Energy Solution, Daejeon, South Korea Jul. 2021-Feb. 2022

Computational Techniques: VASP, Pymatgen, Python, and Shell script

- Analysis of reaction mechanisms in Solid-State Batteries:
    - Utilized atomic-scale modeling techniques to analyze reaction mechanisms in solid-state battery materials, with a focus on deep charge/discharge reactions in Li-Ni-O_2 systems.
- Development of thermodynamic-based analytical methods:
    - Developed thermodynamic-based analytical methods using Python programming, to investigate reaction mechanisms at the interface of battery materials. Presented findings at the LG Tech Conference 2021.
- Development of data collection modules:
    - Created modules for collecting first-principles data from open-source databases and integrating in-house calculations. Facilitated collaborative usage within the team and enhanced research efficiency.
    - Implemented pre- and post-processing techniques to prepare the first-principles calculations for further simulation processes, facilitating collaborative usage and enhancing efficiency in research workflows.

Career break for maternity leave Jun. 2019-Jun. 2021

Post-doctoral Fellow, Seoul National University, Seoul, South Korea Jun. 2016-May 2019

Computational Techniques: VASP, Pymatgen, Ab-initio Molecular dynamics, Defect and Surface Calculation, and Materials Studio, numerical analysis (Pair distribution function analysis, Maxwell-Boltzmann distribution, partial distribution function etc)

- Secured research funding:
    - Obtained $2.5M in research funding from the Korea Research Fellowship, supporting a 5-year research project from 2016 to 2021
- In-Depth investigations of solid electrolyte materials:

    - Conducted comprehensive investigations into the structural properties of sulfide-based solid electrolyte materials, particularly focusing on ensuring their-super-ionic conductivities. Utilized data from ab-initio Molecular Dynamic (AIMD) calculations.
- Investigated Li ion diffusion mechanisms on surface of $Li_7La_3Zr_2O_{12}$:
    - Explored the intricate Li-ion diffusion mechanisms occurring on different surface of $Li_7La_3Zr_2O_{12}$, a prominent solid electrolyte material.
    - Analyzed the implications of Li-ion diffusion behavior for the overall conductivity and performance of $Li_7La_3Zr_2O_{12}$-based solid electrolytes.
    - Conducted in-depth investigations using advanced computational modeling techniques to elucidate the kinetics and pathways of Li-ion diffusion at the surface level.
- Development of numerical analysis methods:
    - Developed various numerical analysis methods to comprehensively understand kinetic properties using a large dataset from ab-initio Molecular Dynamics (AIMD) calculation results.
    - Applied these methods in the $Li_{10}GP_2S_{12}$ and $Na_{11}Sn_2PS_{12}$ project to analyze and interpret complex kinetic phenomena in solid-state materials. Successfully published research findings in a high-impact journal.
- Investigated surface nature and growth mechanisms:
    - Explored the surface nature of host materials and their correlation with the growth mechanism of the poly-lithium sulfides in Li-S batteries.
- Leadership in collaborative projects:
    - Led computational modeling efforts in collaborative projects involving various electrode and solid-electrolyte materials, facilitating interdisciplinary research efforts and fostering advancements.

Post-doctoral Researcher, University of California, Santa Barbara, CA Jun. 2015-Jun. 2016

Computational Techniques: VASP, MATLAB, Cluster Expansion and Numerical analysis (PDF, vector, and integration)

- Conducted in-depth investigation into the phase stabilities of ternary (Li-S-P) compounds and quaternary (Li-S-P-M, M=Ti,Co,Fe) compounds.
- Utilized advanced computational techniques to analyze the phase diagrams and identify stable phase under different conditions.
- Estimated electrochemical phase stabilities of ternary and quaternary compounds using grand canonical energy calculation.

Research Assistant, University of Michigan, Ann Arbor, MI Sep. 2010-May 2015

Computational Techniques: VASP, CASM, Cluster Expansion, Monte Carlo simulation, C++, MTLAB, Shell script, gnu plot, awk, git-hub, and numerical analysis (PDF, (inverse)FFT, integration ,vector etc.)

- Pioneered the development of a ternary cluster expansion and conducted Monte Carlo simulations on conversion battery materials to investigate macroscopic material properties during (de-)lithiation processes.

- Created MATLAB modules to visualize numeric Monte Carlo simulation results, enabling intuitive interpretation of thermodynamic properties and facilitating data analysis.
- Contributed to the development of basic functions within the CASM (A Clusters Approach to Statistical Mechanics) software packages, enhancing computational capabilities in constructing effective Hamiltonians and its utility for research in the field of computational chemistry. Developed functions for defining Space groups, Wyckoff positions, and (inverse-)Fourier Transformations.
- Elucidated the origins of phase transformation hysteresis during electrochemical cycling of the Li-Sb electrode.
- Participated as the leader of computational modeling in several collaborative projects of various electrode materials.
- Investigated the intrinsic properties that facilitate reversibility and minimize the hysteresis during charge and discharge of a Li-Cu-Sb system.
- Revealed the irreversible phase transformation mechanism of TiO_2(B) upon Li discharge
- Identified the electrochemistry of novel intercalation host materials for Li-ion and Na-ion batteries.

Undergraduate research assistant, University of California, Davis, CA Jan. 2009-Aug. 2010

Computational Techniques: MATLAB and Mathematica

- Synthesized ZnO nanoparticle-polymeric thin films and explored their mechanical properties

Teaching Experience

Teaching Assistant, University of Michigan, Ann Arbor, MI Winter Semester 2013

- Introduction to Materials and Manufacturing (MSE 220, Core class)
- Instructed the discussion section and held weekly office hours and graded problem sets and tests

EDITORIAL WORK

Journals Reviewed

- *Chemistry of Materials*
- *ACS Applied Materials & Interfaces*
- *Nano Energy*
- *Journal of Materials Chemistry A*

TECHNICAL EXPERTISE

Software

- VASP
- Pymatgen
- Materials Studio
- Materials Projects
- CASM
- MATLAB

Multiscale Modeling of Materials Techniques

- Cluster expansion
- Grand canonical Monte Carlo
- Machine Learning
- Phase stability
- Ab-initio Molecular dynamics
- Surface energy calculation
- Defects

- Reaction between Solid-Solid Interface (Reaction energy, Electrochemical stability)
- Diffusion Mechanism

Materials Characterization

- XRD (Rigaku SmartLab, Rigaku Ultima III)
- TGA-DSC (Netzsch simultaneous thermal analyzer STA 449 F3 Jupiter)
- SEM (FIB Quanta 3D)

Electrochemical Techniques

- Electrochemical Impedance Spectroscopy (EIS)
- Cyclic Voltammetry (CV)

Certifications

- Battery State-of-Charge (SoC) Estimation, Coursera, July 2023
- Equivalent Circuit Cell Model Simulation, Coursera, Jun 2023
- Introduction to battery-management systems, Coursera, June 2023
- Machine Learning, Coursera, June 2019

PUBLICATIONS (total publications: 14, h-index: 11, total citations 847, Google Scholar Link)

(∗ equal contribution)

- Sung Joo Kim, Jae Yeol Park, Yoonsu Shim, **Donghee Chang**, Joon Ha Chang, Kyun Seong Dae, and Jong Min Yuk. "Microscopic Insight Into Tin Nanoparticle Magnesiation", *ACS Applied Energy Material*, 5(7):7944-7949 (2022)
- Sung-Kyun Jung∗, Insang Hwang∗, **Donghee Chang∗**, Kyu-Young Park∗, Sung Joo Kim, Won Mo Seong, Donggun Eum, Jooha Park, Byunghoon Kim, Jihyeon Kim, Jae Hoon Heo, and Kisuk Kang," Nanoscale phenomena in lithium-ion battereis," *Chemical Reviews*, 120(14):6684-6737 (2019)
- Myeong Hwan Lee, Sung Joo Kim, **Donghee Chang**, Jinsoo Kim, Sehwan Moon, Kyungbae Oh, Kyu-Young Park, Won Mo Seong, Hyeokjun Park, Giyun Kwon, Byungju Lee, and Kisuk Kang, "Toward a low-cost high-voltage sodium aqueous rechargeable battery", *Materials Today*, 29:26-36(2019)
- Zheng-Long Xu*, Sung Joo Kim*, **Donghee Chang***, Kyu-Young Park, Kyun Seong Dae, Khoi Dao, Jong Min Yuk, and Kisuk Kang," Visualization of regulated nucleation and growth of lithium sulfides for high energy lithium sulfur batteres," *Energy & Environmental Science* 12(10):3144-3155 (2019)
- Kyungbae Oh, **Donghee Chang**, Inchul Park, Kyungho Yoon, and Kisuk Kang, "First-Principles Investigations on Sodium Superionic Conductor $Na_{11}Sn_2PS_{12}$", *Chemistry of Materials*, 31(16):6066-6075(2019)
- **Donghee Chang**, Kyungbae Oh, Sung Joo Kim, and Kisuk Kang," Super-Ionic Conduction in Solid-State Li7P3S11-Type Sulfide Electrolytes," *Chemistry of Materials*, 30(24):8764-8770 (2018)
- Kyungbae Oh, **Donghee Chang**, Byungju Lee, Do-Hoon Kim, Gabin Yoon, Inchul Park, Byunghoon Kim, and Kisuk Kang, "Native Defects in $Li_{10}GeP_2S_{12}$ and Their Effect on Lithium Diffusion", *Chemistry of Materials*, 30(15):4995-5004 (2018)

- Sung Joo Kim*, **Donghee Chang***, Kui Zhang, George Graham, Anton Van der Ven, and Xiaoqing Pan," Accordion Strain Accommodation Mechanism within the Epitaxially Constrained Electrode," *ACS Energy Letters*, 3(8):1848-1853 (2018)
- Gabin Yoon, Do-Hoon Kim, Inchul Park, **Donghee Chang**, Byunghoon Kim, Byungju Lee, Kyungbae Oh, and Kisuk Kang, " Using Frist-Principles Calculations for the Advancement of Materials for Rechargeable Batteries", *Advanced Functional Materials*, 27(40):1702887 (2017)
- **Donghee Chang** and Anton Van der Ven," Li intercalation mechanisms in $CaTi_5O_{11}$, a bronze-B derived compound," *Physical Chemistry Chemical Physics*, 18(47):32042-32049 (2016)
- **Donghee Chang**, Min-Hua Chen, and Anton Van der Ven," Factors Contributing to Path Hysteresis of Dis- placement and Conversion Reactions in Li Ion Batteries," *Chemistry of Materials*, 27(22):7593-7600 (2015)
- **Donghee Chang**, Hua Huo, Karen E. Johnston, Michel Menetrier, Laure Monconduit, Clare P. Grey, and Anton Van der Ven," Elucidating the Origins of Phase Transformation Hysteresis During Electrochemical Cycling of Li-Sb electrodes," *Journal of Materials Chemistry A*, 3(37):18928-18943 (2015)
- Jue Liu, **Donghee Chang**, Pamela Whitfield, Yuri Janssen, Xiqian Yu, Yongning Zhou, Jianming Bai, Jonathan Ko, Kyung-Wan Nam, Lijun Wu, Yimei Zhu, Mikhail Feygenson, Glenn Amatucci, Anton Van der Ven, Xiao- Qing Yang, and Peter Khalifah," Ionic Conduction in Cubic $Na_3TiP_3O_9N$, a Secondary Na-Ion Battery Cath- ode with Extremely Low Volume Change," *Chemistry of Materials*, 26(10):3295-3305 (2014)
- Kenneth J Loh, and **Donghee Chang**,"Zinc oxide nanoparticle-polymeric thin films for dynamic strain sensing", *Journal of Materials Science*, 46:228-237 (2011)