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RESEARCH INTERESTS

Atomistic Modelling, Density Functional Theory Calculations, Molecular Dynamics, Large Scale Computation
Energy Storage Materials, Solid-state Batteries, Multi-valent Batteries.

PROFESSIONAL EXPERIENCES & AFFILIATIONS

Chung-Ang University, Seoul, South Korea *Sep. 2021– Present*
Assistant Professor, School of Integrative Engineering

Argonne National Laboratory (ANL), Lemont, IL *Feb. 2019– Aug. 2021*
Postdoctoral Appointee, Materials Science Division
Mentor: Dr. Peter Zapol

EDUCATION

University of Michigan – Ann Arbor, MI *Sep. 2013– Dec. 2018*
PhD in Mechanical Engineering
Advisor: Professor Donald J. Siegel

Master of Science in Engineering (MSE) in Mechanical Engineering
Advisor: Professor Donald J. Siegel

Seoul National University, South Korea *Mar. 2006– Feb. 2013*
Bachelor of Science (BS) in Mechanical and Aerospace Engineering
Graduated with honors (Cum laude)

PUBLICATIONS

Note: # indicates equally contributed authors, * represents corresponding authors

- [1] S. Kim, L. Yin, S.-M. Bak, T. T. Fister, **H. Park**, P. Parajuli, J. Gim, Z. Yang, R. F. Klie, P. Zapol, Y. Du, S. H. Lapidus, J. T. Vaughney*
"Investigation of Ca Insertion into α -MoO₃ Nanoparticles for High Capacity Ca-Ion Cathodes"
Nano Letters **22**, 2228-2235 (2022). 10.1021/acs.nanolett.1c04157
- [2] **H. Park***, C. J. Bartel, G. Ceder, P. Zapol*
"Layered Transition Metal Oxides as Ca Intercalation Cathodes: A Systematic First-Principles Evaluation"
Advanced Energy Materials **11**, 2101698 (2021). 10.1002/aenm.202101698
- [3] A. Das, **H. Park**, Y. Chen, D. Choudhury, T.-L. Lee, J. W. Elam, P. Zapol, M. J. Bedzyk*
"Atomic-Scale Structure of Chemically Distinct Surface Oxygens in Redox Reactions"
Journal of the American Chemical Society **143**, 17937-17941 (2021). 10.1021/jacs.1c07926
- [4] **H. Park**, S. Yu, D. J. Siegel*
"Predicting Charge Transfer Stability between Sulfide Solid Electrolytes and Li Metal Anodes"
ACS Energy Letters **6**, 150-157 (2021). 10.1021/acsenerylett.0c02372

- [5] P. Parajuli*#, **H. Park#**, B. J. Kwon, J. Guo, B. Key, J. T. Vaughey, P. Zapol, R. F. Klie*
"Direct Observation of Electron Beam-Induced Phase Transition in MgCrMnO₄"
Chemistry of Materials **32**, 10456-10462 (2020). 10.1021/acs.chemmater.0c03121
- [6] **H. Park***, P. Zapol*
"Thermodynamic and kinetic properties of layered-CaCo₂O₄ for the Ca-ion batteries: a systematic first-principles study"
Journal of Materials Chemistry A **8**, 21700-21710 (2020). 10.1039/D0TA07573F
- [7] S. Kim, L. Yin, M. H. Lee, P. Parajuli, L. Blanc, T. T. Fister, **H. Park**, B. J. Kwon, B. J. Ingram, P. Zapol, R. F. Klie, K. Kang, L. F. Nazar*, S. H. Lapidus, J. T. Vaughey*
"High-Voltage Phosphate Cathodes for Rechargeable Ca-Ion Batteries"
ACS Energy Letters **5**, 3203-3211 (2020). 10.1021/acscenergylett.0c01663
- [8] L. Hu, J. R. Jokisaari, B. J. Kwon, L. Yin, S. Kim, **H. Park**, S. H. Lapidus, R. F. Klie, B. Key, P. Zapol, B. J. Ingram, J. T. Vaughey, J. Cabana*
"High Capacity for Mg²⁺ Deintercalation in Spinel Vanadium Oxide Nanocrystals"
ACS Energy Letters **5**, 2721-2727 (2020). 10.1021/acscenergylett.0c01189
- [9] B. J. Kwon*, L. Yin, **H. Park**, P. Parajuli, K. Kumar, S. Kim, M. Yang, M. Murphy, P. Zapol, C. Liao, T. T. Fister, R. F. Klie, J. Cabana, J. T. Vaughey, S. H. Lapidus, B. Key*
"High Voltage Mg-Ion Battery Cathode via a Solid Solution Cr–Mn Spinel Oxide"
Chemistry of Materials **32**, 6577-6587 (2020). 10.1021/acs.chemmater.0c01988
- [10] D. Park, **H. Park**, Y. Lee, S.-O. Kim, H.-G. Jung, K. Y. Chung, J. H. Shim, S. Yu*
"Theoretical Design of Lithium Chloride Superionic Conductors for All-Solid-State High-Voltage Lithium-Ion Batteries"
ACS Applied Materials & Interfaces **12**, 34806-34814 (2020). 10.1021/acscami.0c07003
- [11] D. Xu, E. M. Hopper, K.-C. Chang, P. M. Baldo, **H. Park**, J. A. Eastman, H. You, P. H. Fuoss, B. J. Ingram*, P. Zapol*
"The effect of water vapor on surface oxygen exchange kinetics of thin film (La,Sr)(Co,Fe)O_{3-δ}"
Journal of Power Sources **451**, 227478 (2020). 10.1016/j.jpowsour.2019.227478
- [12] **H. Park**, Y. Cui, S. Kim, J. T. Vaughey, P. Zapol*
"Ca Cobaltites as Potential Cathode Materials for Rechargeable Ca-Ion Batteries: Theory and Experiment"
The Journal of Physical Chemistry C **124**, 5902-5909 (2020). 10.1021/acs.jpcc.9b11192
- [13] B. J. Kwon, K.-C. Lau, **H. Park**, Y. A. Wu, K. L. Hawthorne, H. Li, S. Kim, I. L. Bolotin, T. T. Fister, P. Zapol, R. F. Klie, J. Cabana, C. Liao, S. H. Lapidus, B. Key*, J. T. Vaughey*
"Probing Electrochemical Mg-Ion Activity in MgCr_{2-x}V_xO₄ Spinel Oxides"
Chemistry of Materials **32**, 1162-1171 (2020). 10.1021/acs.chemmater.9b04206
- [14] S. Yu*, **H. Park**, D. J. Siegel*
"Thermodynamic Assessment of Coating Materials for Solid-State Li, Na, and K Batteries"
ACS Applied Materials & Interfaces **11**, 36607-36615 (2019). 10.1021/acscami.9b11001
- [15] **H. Park#**, N. Kumar#, M. Melander#, T. Vegge, J. M. Garcia Lastra, D. J. Siegel*
"Adiabatic and Nonadiabatic Charge Transport in Li–S Batteries"
Chemistry of Materials **30**, 915-928 (2018). 10.1021/acs.chemmater.7b04618
- [16] **H. Park**, D. J. Siegel*
"Tuning the Adsorption of Polysulfides in Lithium–Sulfur Batteries with Metal–Organic Frameworks"
Chemistry of Materials **29**, 4932-4939 (2017). 10.1021/acs.chemmater.7b01166
- [17] **H. Park**, H. S. Koh, D. J. Siegel*
"First-Principles Study of Redox End Members in Lithium–Sulfur Batteries"
The Journal of Physical Chemistry C **119**, 4675-4683 (2015). 10.1021/jp513023v

- [18] B. Lee, **H. Park**, H. Bang*
"Multidirectional Pointing Input Using a Hardware Keyboard"
ETRI Journal **35**, 1160-1163 (2013). 10.4218/etrij.13.0213.0117

AWARDS/FELLOWSHIPS

- ACS 'Most Read Article' designation**, Chemistry of Materials, American Chemical Society *May. 2017*
- William Mirsky Memorial Fellowship**, Department of Mechanical Engineering, University of Michigan *Apr. 2014*
- Overseas Scholarship**, Kwanjeong Educational Foundation
Granted \$110,000 during Graduate study *Sep. 2013*
- The Best Presentation Award for Bachelor Thesis Presentation Contest**, School of Mechanical & Aerospace Engineering, SNU *Nov. 2012*
- National Science and Engineering Undergraduate Scholarship**, National Research Foundation of Korea
Granted Full Tuitions during Undergraduate Study *Mar. 2006*

Grant

- National Research Foundation of Korea, Young Researcher Program, "Development of Ca Intercalation Electrode Materials for Ca-ion Battery using Density Functional Theory Calculations", 431,535K KRW (~360K USD), Park is PI *Mar. 2022– Mar. 2025*
- Chung-Ang University, New Faculty Grant, 15,000K KRW (~13K USD), Park is PI *Sep. 2021– Sep. 2023*
- National Energy Research Scientific Computing Center (NERSC), "Search for novel electrode materials for multivalent batteries through high-throughput computing", 10,000,000 NERSC hours, Park is PI *Jan. 2021– Jan. 2022*
- Argonne National Laboratory, "First Principles Study of Multivalent Cathodes", 2,800,000 CPU hours, Park is PI *Apr. 2019– Oct. 2021*

PRESENTATIONS

- [1] (Oral) "First-Principles Study of Layered Transition Metal Oxides As a Cathode Material for Ca-Ion Intercalating Batteries", A02: Multivalent Batteries, PRiME, Honolulu, HI, US, Oct. 2020 (Converted to online events due to COVID-19)
- [2] (Poster) "Calcium Cobaltites as Potential Cathode Materials for Rechargeable Ca Ion Batteries", Gordon Research Conference on Batteries, Ventura, CA, US, Feb. 2020
- [3] (Oral) "Band Edge Considerations for Interfacial Stability Between Sulfide Solid Electrolytes and Li Metal Anodes" ET01: Solid-State Batteries—Materials, Interfaces and Performance, 2018 MRS Fall Meeting, Boston, MA, US, Nov. 2018
- [4] (Oral) "Tuning the Adsorption of Polysulfides (Li_2S_n) in Lithium-Sulfur Batteries with Metal-Organic Frameworks(MOFs)" A03: Li-ion Batteries and Beyond, 233rd ECS Meeting, Seattle, WA, US, May 2018
- [5] (Oral) "Adiabatic and Nonadiabatic Charge Transport in Li-S Batteries" L04: Charge Transfer: Electrons, Protons, and Other Ions 3, 233rd ECS Meeting, Seattle, WA, US, May 2018
- [6] (Poster) "Tuning Polysulfide Adsorption in Li-S Positive Electrodes with Metal Organic Frameworks" Poster session, PRiME, Honolulu, HI, US, Oct. 2016
- [7] (Poster) "Charge Transport Mechanism in Solid-State Redox-End Members in Lithium-Sulfur (Li-S) Batteries" Poster session, PRiME, Honolulu, HI, US, Oct. 2016
- [8] (Poster) "First-Principles Study of Redox End-Members in Lithium-Sulfur Batteries" Poster session, 2014 MRS Fall Meeting, Boston, MA, US, Dec. 2014

PATENTS

1. Korea Patent "*Easy tie - Tying hair with one hand*", Nov. 2012
2. Korea Patent "*Latch Structure for Door could only be pulled*", May. 2012

SERVICE to PROFESSIONAL ORGANIZATIONS

Chaired Symposium

PRiME 2020, A02 - Multivalent Batteries 2, Honolulu, HI, US, Oct. 2020

Reviewers: International Journal of Energy Research, Computational and Theoretical Chemistry, Physica E