Haesun Park, **Ph.D.**

Assistant Professor

Chung-Ang University, School of Integrative Engineering, Seoul, Republic of Korea, 06974

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RESEARCH INTERESTS

Atomistic Modelling, Density Functional Theory Calculations, Molecular Dynamics, Large Scale Computation

AI Accelerated High-Throughput Simulations, Active Learning, Lab Automation

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] H.J. Kim#, H. Li#, D. Kim#, G. Park, S.E. Jo, K. Ju, Y. Kwon, **H. Park***, M.H. Kee*, J. An*
"Active and Stable Plasma-Enhanced ALD Pt@Ni-YSZ Hydrogen Electrode for Steam Reversible Solid Oxide Cells"
Applied Catalysis B: Environment and Energy, Accepted

[2] J. Park*, Y. Yang, **H. Park**, A. Sundar, S. Lee, T. Kinnibrugh, S.-B. Son, E. Lee, P. Zapol, R. Klie, J. J. Kim*
"Entropy-stabilized multi-cation fluorides as conversion-type cathode for Li-ion batteries – impact of element selection"
ACS Applied Materials & Interfaces, ASAP (2024). 10.1021/acsami.4c12920

[3] J. Park, J. Lee, J. Kee, K. Min, **H. Park***, S. Lee*
"Active Learning Framework for Expediting the Search of Thermodynamically Stable MXenes in the Extensive Chemical Space"
ACS Nano, ASAP (2024). 10.1021/acsnano.4c08621

[4] C.Y. Son[#], D. Kim[#], S.-Y. Jun, **H. Park***, W,-H Ryu*
"Asymmetrical Functionalization of Polarizable Interface Restructuring Molecules for Rapid and Longer Operative Lithium Metal Batteries"
Small, 2405143 (2024). 10.1002/smll.202405143

[5] M.J. Kim, **H. Park***
"Computational Screening of Ca-Containing Coating Materials for Electrodes of Ca-Ion Batteries."
International Journal of Energy Research **2024** (2024). 10.1155/2024/7007091

[6] K.-R. Yeo, H. Kim, K.-S. Lee, S. Kim, J. Lee*, **H. Park***, S.-K. Kim*
"Controlled doping of ultralow amounts Ru on Ni cathode for PEMWE: Experimental and theoretical elucidation of enhanced performance"
Applied Catalysis B: Environment and Energy **346**, 123738 (2024). 10.1016/j.apcatb.2024.123738

[7] J. J. Kim*, B. Kc, **H. Park**, A. Sundar, G. Evmenenko, D. B. Buchholz, J. Guo, B. J. Ingram, P. Zapol, R. F. Klie, T. T. Fister
"Strain-Driven Surface Reactivity in Magnesium-Ion Battery Cathodes"
Chemistry of Materials **36**, 1342-1351 (2024). 10.1021/acs.chemmater.3c02490

[8] S. Kim*, N. T. Hahn, T. T. Fister, N. J. Leon, X.-M. Lin, **H. Park**, P. Zapol, S. H. Lapidus, C. Liao, J. T. Vaughey*
"Investigation of Rechargeable Calcium Metal-Selenium Batteries Enabled by Borate-Based Electrolytes"
Chemistry of Materials **35**, 2363-2370 (2023). 10.1021/acs.chemmater.2c03343

[9] 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. Vaughey*
"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

[10] **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

[11] 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

[12] **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/acsenergylett.0c02372

[13] 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

[14] **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

[15] 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/acsenergylett.0c01663

[16] 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/acsenergylett.0c01189

[17] 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

[18] 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/acsami.0c07003

[19] 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)O3-δ"
Journal of Power Sources **451**, 227478 (2020). 10.1016/j.jpowsour.2019.227478

[20] **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

[21] 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 MgCr2–xVxO4 Spinel Oxides"
Chemistry of Materials **32**, 1162-1171 (2020). 10.1021/acs.chemmater.9b04206

[22] 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/acsami.9b11001

[23] **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

[24] **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

[25] **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

[26] 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 — ***Sep. 2013***
Granted $110,000 during Graduate study

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 — ***Mar. 2006***
Granted Full Tuitions during Undergraduate Study

Grant (Park's share of total funds awarded: ~1,500,000K KRW)

Chung-Ang University, Outstanding Early Career Researcher Grant, 10,000K KRW (~8K USD), Park is PI — ***Oct. 2024– Sep. 2025***

National Research Foundation of Korea, Global Basic Research Laboratory, "Laboratory of Advancing Water Electrolysis Electrode using High-Precision Computation", 1,370,000K KRW (~1M USD), Park is PI, my share is 550,000K KRW (~420K USD) — ***Aug. 2024– Jul. 2027***

National Research Council of Science & Technology, Global Top Strategy Research Group Program, "Advanced Battery platform for leading next-generation battery technology", 130,000,000K KRW (~100M USD), Park is co-PI, my share is 500,000K KRW (~400K USD) — ***Jun. 2024– May. 2029***

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_x) 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 ORGANIZAIONS

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