Haesun Park (박해선), **Ph.D.**

Postdoctoral Appointee

Argonne National Laboratory, Materials Science Division, Lemont, IL 60439

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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

Argonne National Laboratory (ANL), Lemont, IL — ***Feb. 2019– Present***
Postdoctoral Appointee, Materials Science Division
Advisor: 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

Lead Authored Papers

[1] **H. Park***, C.J. Bartel, G. Ceder, P. Zapol*
"Layered Transition Metal Oxides as Ca intercalation Cathodes: A Systematic First-principles Evaluation"
submitted (2021).

[2] **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). https://doi.org/10.1021/acsenergylett.0c02372

[3] **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). https://doi.org/10.1039/D0TA07573F

[4] **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). https://doi.org/10.1021/acs.jpcc.9b11192

[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). https://doi.org/10.1021/acs.chemmater.0c03121

[6] **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). https://doi.org/10.1021/acs.chemmater.7b04618

[7] **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). https://doi.org/10.1021/acs.chemmater.7b01166

[8] **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). https://doi.org/10.1021/jp513023v

Contributing Authored Papers

[1] 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). https://doi.org/10.1016/j.jpowsour.2019.227478

[2] 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). https://doi.org/10.1021/acs.chemmater.0c01988

[3] 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). https://doi.org/10.1021/acs.chemmater.9b04206

[4] 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). https://doi.org/10.1021/acsenergylett.0c01663

[5] 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). https://doi.org/10.1021/acsenergylett.0c01189

[6] 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). https://doi.org/10.1021/acsami.9b11001

[7] B. Lee, **H. Park**, H. Bang*
"Multidirectional Pointing Input Using a Hardware Keyboard"
ETRI Journal **35**, 1160-1163 (2013). https://doi.org/https://doi.org/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

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