

Curriculum Vitae

HOJE CHUN

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RESEARCH/PROFESSIONAL EXPERIENCES

- Postdoctoral Fellow** (*Advisor*: Prof. Rafael Gómez-Bombarelli) *Oct. 2023*
~ *Present*
Department of Materials Science and Engineering,
Massachusetts Institute of Technology, Boston, USA
- Postdoctoral Associate** (*Advisor*: Prof. Byungchan Han) *Mar. 2023*
~ *Present*
BK21 Postdoc, Department of Chemical and Biomolecular Engineering,
Center of Converged Energy Materials Research (CEMRC)
Yonsei University, Seoul, Korea
- Visiting Graduate Student Researcher** (*Advisor*: Prof. Rafael Gómez-Bombarelli) *July 2022*
~*Sep. 2022*
Department of Materials Science and Engineering,
Massachusetts Institute of Technology, Boston, USA

EDUCATION

- Yonsei University**, Seoul, Korea *Mar. 2018*
~ *Feb. 2023*
Ph.D. in the Department of Chemical and Biomolecular Engineering
Thesis: Machine Learning Accelerated First-Principles Design of High Functional Energy
Conversion and Storage Materials
Advisor: Prof. Byungchan Han, Department of Chemical and Biomolecular Engineering
- Yonsei University**, Seoul, Korea *Mar. 2014*
~ *Feb. 2018*
B.Eng. in Energy and Environmental Science and Engineering

RESEARCH INTERESTS

Machine-learning atomic potentials & high-throughput virtual screening

Nanomaterials: investigation of nanoparticles dynamics and their functionalities

Sustainable & energy materials: first-principles calculations of functional materials

HONORS & AWARDS

- BK 21 Plus Postdoctoral Scholarship, Yonsei University *2023-2024*
- Program of Fostering Global Leaders for Innovative Growth Industry *2023-2024*
- Global Ph.D. Fellowship, The National Research Foundation of Korea (NRF)** *2019-2023*
- Best Poster Award, The Korean Institute of Surface Engineering *24 June 2022*
- Best Poster Award, The Korean Institute of Chemical Engineers *28 Oct. 2022*
- Best Poster Award, The Korean Institute of Metals and Materials *21 Nov. 2021*
- BK21 Graduate Student Award, Yonsei University *04 Feb. 2021*
- Best Poster Award (Gold Medal), Nano Korea 2019 *05 July 2019*

First author papers:

16. **H. Chun**, J. R. Lunger, R. Gómez -Bombarelli*, and B. Han*, "Active learning accelerated exploration of atomic level catalytic tunability in multi-metallic single atom catalysts for oxygen electrocatalysis", In preparation
15. **H. Chun**+, J. Kang+, D. Kang, S. J. Hong, M. Hong, J. Heo, B. H. Kim*, J. Park*, B. Han*, "Structural dynamics and individual site catalytic activity of ligand protected platinum nanoparticles", In preparation
14. J. Lee+, X. A. Le+, **H. Chun**+, T. H. Vu, D. Choi, B. Han*, M. I. Kim*, and J. Lee*, Active site engineering of Zn-doped mesoporous ceria toward highly efficient organophosphorus hydrolase-mimicking nanozyme, *Biosensors and Bioelectronics*, Submitted
13. D. G. Park+, J. W. Choi+, **H. Chun**+, H. S. Jang, H. Lee, W. H. Choi, B. C. Moon, K-H. Kim, M. G. Kim, B. Han*, K. M. Choi*, and J. K. Kang*, "Increasing CO binding energy and defects by preserving Cu oxidation state via O₂ plasma-assisted N doping on CuO enables high C₂₊ selectivity and long-term stability in electrochemical CO₂ reduction", *ACS Catalysis*, 13, 9222-9233 [[Link](#)]
12. S. Hyun+, **H. Chun**+, M. Hong, J. Kang, and B. Han*, First-principles Study on Ultrafast Li-ion Diffusion in Halospinel Li₂Sc_{2/3}Cl₄ through Multichannel Designed by Alivalent Dopants, *Journal of Materials Chemistry A*, (2023) 11, 8, 4272-4279 [[Link](#)]
11. S. W. Koh+, J. Hu+, **H. Chun**+, P. Yu+, J. Ge, Z. Sun, W. Hong, Q. Liu, K. Nam, B. Han*, Z. Liu*, H. Li*, "Two-dimensional palladium phosphoronitride for enhanced oxygen reduction reaction", *Applied Materials & Interfaces*, (2022)14, 10, 12156-12167 [[Link](#)]
10. D. K. Yesudoss+, **H. Chun**+, B. Han*, S. Shanmugam*, "Accelerated N₂ reduction kinetics via Synergistic Charge Transfer in Hybrid NbTiO₄ electrocatalyst", *Applied Catalysis B: Environmental*, (2021) 304, 120938 [[Link](#)]
9. **H. Chun**+, E. Lee+, K. Nam, JH. Jang, W. Kyoung, S. H. Noh*, B. Han*, "First-principles Data Integrated Machine-learning Approach for High-throughput Searching of Ternary Electrocatalyst towards Oxygen Reduction Reaction", *Chem Catalysis*, (2021) 1, 4, 855-869 (Front Cover) [[Link](#)]
8. S. J. Hong+, **H. Chun**+, J. Lee, B.H. Kim, M. H. Seo, J. Kang*, B. Han*, "First-Principles Based Machine-Learning Molecular Dynamics for Crystalline Polymers with Van der Waals Interactions", *Journal of Physical Chemistry Letters*, (2021) 12, 25, 6000-6006 (Front Cover) [[Link](#)]
7. **H. Chun**+, K. Nam, S. J. Hong, J. Kang*, B. Han*, "Design of a Unique Anion Framework in Halospinel for Outstanding Performance of All Solid-state Li-ion Battery: First-principles Approach", *Journal of Materials Chemistry A*, (2021) 9, 15605-15612 [[Link](#)]
6. **H. Chun**+, D. Choi+, J. Kang, J. S. Park, B. Han*, "First-principles computational study of Ni/ α -Al₂O₃ hybrid interface reactions under extreme thermodynamic conditions", *Applied Surface Science*, (2020) 509, 144861 [[Link](#)]
5. K. Nam+, **H. Chun**+, J. Hwang, B. Han*, "First-principles design of highly functional sulfide electrolyte of Li_{10-x}SnP₂S_{12-x}Cl_x for all solid-State Li-ion battery applications", *ACS Sustainable Chemistry & Engineering*, (2020) 8, 8, 3321-3327 [[Link](#)]
4. GY. Cha+, **H. Chun**+, DY. Hong+, J. Kim, KH. Cho, UH. Lee, JS. Chang, S. G. Ryu*, H. W. Lee, SJ. Kim*, B. Han*, Y. K. Hwang*, "Unique design of superior metal-organic framework for removal of toxic chemicals in humid environment via direct functionalization of the metal nodes", *Journal of Hazardous Materials*, (2020) 398, 122857 [[Link](#)]
3. K. Ho+, **H. Chun**+, H. C. Lee, Y. Lee, S. Lee, H. Jung, B. Han*, CH. Lee, "Design of highly efficient

adsorbents for removal of gaseous methyl iodide using tertiary amine-impregnated activated carbon: Integrated experimental and first-principles approach", *Chemical Engineering Journal*, (2019) 373, 1003-1011 [[Link](#)]

2. **H. Chun**, J. Kang, B. Han*, "Universal scaling relationship to screen an efficient metallic adsorbent for adsorptive removal of iodine gas under humid conditions: first-principles study", *Journal of Physical Chemistry C*, (2018) 122, 22, 11799-11806 [[Link](#)]
1. **H. Chun**, J. Kang, B. Han*, "First principles computational study on the adsorption mechanism of organic methyl iodide gas on triethylenediamine impregnated activated carbon", *Physical Chemistry Chemical Physics*, (2016) 18, 32050-32056 [[Link](#)]

Co-author papers:

23. S. Kang+, J. Kim+, S. Kim, **H. Chun**, J. Heo, C. F. Reboul, C. Machello, M. Lee, D. Kang, B. H. Kim, T. Hyeon, B. Han*, P. Ercius*, H. Elmlund*, and J. Park*, "Single nanocrystal etching by 4D graphene liquid cell electron microscopy", In preparation
22. M. Hong, **H. Chun**, S. Noh, and B. Han*, "Learning pairwise interaction in multi-component interatomic potentials using physically-informed neural network", In preparation
21. J. R. Lunger, J. Karaguesian, **H. Chun**, J. Peng, Y. Tseo, C. H. Shan, B. Han, Y. Shao-Horn*, and R. Gómez-Bombarelli*, "Atom-by-atom designs of metal oxide catalysts for the oxygen evolution reaction", *npj Computational Materials*, Submitted
20. J-H. Kim, J. Kim, B. H. Kim, S. Song, **H. Chun**, H. Choi, H. Cho, J. W. Jung, Y. Sohn, J. Jeong, K. Park, S. Jeon, B. Han, W. C. Lee, J. Kang, M. Lee, T. Hyeon, J. Sung, J. Park*, Multiphase growth dynamics of nanoparticle ensembles, *Journal of the American Chemical Society*, Submitted
19. T. Wei, **H. Chun**, S. Hyun, B. Han*, Design a multiphase interfaced Ge(GeO_x)/T-Nb₂O_{5-x}/C anode with synergistic high capacity and durability for Li-ion batteries, *Applied Surface Science*, (2023) 158424 [[Link](#)]
18. J. Heo+, D. Kim+, H. Choi+, S. Kim, **H. Chun**, C. F. Reboul, C. T. S. Van, D. Elmlund, S. Choi, K. Kim, Y. Park, H. Elmlund*, B. Han*, and J. Park*, "Method for 3D atomic structure determination of multi-element nanoparticles with graphene liquid-cell TEM", *Scientific Reports*, (2023) 13, 1814 [[Link](#)]
17. M. Liu, **H. Chun**, TC. Yang, S. J. Hong, CM. Yang*, B. Han*, L. YS. Lee*, Tuning the site-to-site interaction in Ru-M (M = Co, Fe, Ni) di-atomic electrocatalysts to climb up the volcano plot of oxygen electroreduction, *ACS Nano*, (2022) 16 (7), 10657-10666 [[Link](#)]
16. S. J. Hong, **H. Chun**, M. Hong, B. Han*, "N- and B-doped fullerene as peroxidase- and catalase- like metal-free nanozymes with pH-switchable catalytic activity: a first-principles approach", *Applied Surface Science*, (2022) 598, 153715 [[Link](#)]
15. J. Choi+, D. Kim+, S. J. Hong+, X. Zhang, H. Hong, **H. Chun**, B. Han*, L. YS. Lee*, Y. Piao*, Tuning the electronic structure and inverse degree of inverse spinel ferrites by integrating samarium orthoferrite for efficient water oxidation, *Applied Catalysis B: Environmental*, (2022) 315, 121504 [[Link](#)]
14. J. Heo, D. Kang, S. Kim, **H. Chun**, B. Han*, B. H. Kim*, Jungwon Park*, "3-Dimensional Scanning of Entire Unit Cells in Single Nanoparticles", *ChemNanoMat*, (2022), e202200057, 1-7 [[Link](#)]
13. M. Hong, **H. Chun**, C. Kwon, B. Han*, Outstanding Stability of Gd-doped UO₂ against Surface Oxidation: First-principles Study, *Applied Surface Science*, (2022), 589, 152955 [[Link](#)]
12. J. Hong, JW Bae, H. Jo, HY. Park, S. Lee, S. J. Hong, **H. Chun** et al., "Metastable Hexagonal Close-Packed Palladium Hydride in Liquid Cell Transmission Electron Microscopy", *Nature*, (2022), 603, 631-636. [[Link](#)]
11. J. Park+, JM. Lee+, **H. Chun**, Y. Lee, S. J. Hong, H. Jung, YJ. Kim, WG. Kim, V. Devaraj, E. J. Choi, JW. Oh*, B. Han*, "Optical bioelectronic nose of outstanding sensitivity and selectivity toward volatile organic compounds implemented with genetically engineered bacteriophage: Integrated study of multi-scale

- computational prediction and experimental validation", *Biosensors & Bioelectronics*, (2021) 177, 112979 [[Link](#)]
10. JM. Lee⁺, J. W. Choi⁺, I. Jeon⁺, Y. Zhu, T. Yang, **H. Chun**, J. Shin, J. Park, J. Bang, K. Lim, WG. Kim, Y. Kim, H. Jeong, E. J. Choi, V. Devaraj, J. S. Nam, H. Ahn, YC. Kang, B. Han*, M. Song*, JW. Oh*, Chuanbin Mao*, "High quantum efficiency and stability of biohybrid quantum dots nanojunctions in bacteriophage-constructed perovskite", *Materials Today Nano*, (2021) 13, 100099 [[Link](#)]
 9. S. J. Hong, **H. Chun**, C. Kwon, B. Han*, "n-Type thermoelectric properties of a hexagonal SiGe polymorph superior to a cubic SiGe", *Journal of Alloys and Compounds*, (2021) 874, 160007 [[Link](#)]
 8. K. Nam, **H. Chun**, J. Hwang, K. A. Min, B. Han*, "Pairing of Transition Metal Dichalcogenides and Doped Graphene for Catalytically Dual Active Interfaces for the Hydrogen Evolution Reaction", *ACS Sustainable Chemistry & Engineering*, (2020) 8, 29, 10852-10858 (Supplementary Back Cover) [[Link](#)]
 7. S. J. Hong, **H. Chun**, K. A. Min, B. Han*, "First-principles mechanism study on distinct optoelectronic properties of Cl-doped 2D hybrid tin iodide perovskite", *Journal of Materials Chemistry C*, (2020) 8, 9540-9548 (Back Cover) [[Link](#)]
 6. B. H. Kim⁺, J. Heo⁺, S. Kim, C. F. Reboul, **H. Chun**, D. Kang, H. Bae, H. Hyun, J. Lim, H. Lee, B. Han, T. Hyeon, A. P. Alivisatos, P. Ercius*, H. Elmlund*, J. Park*, "Critical differences in 3D atomic structure of individual ligand-protected nanocrystals in solution", *Science*, (2020) 368, 60-67 (Front Cover) [[Link](#)]
 5. Y. Zhao⁺, J. Hwang⁺, M. T. Tang, **H. Chun**, X. Wang, H. Zhao, K. Chan, B. Han*, P. Gao*, H. Li*, "Ultrastable molybdenum disulfide-based electrocatalyst for hydrogen evolution in acidic media", *Journal of Power Sources*, (2020) 456, 227998 [[Link](#)]
 4. H. Jung, J. Hwang, **H. Chun**, B. Han*, "Elucidation of hydrolysis reaction mechanism of tungsten hexafluoride (WF₆) using first-principles calculations", *Journal of Industrial and Engineering Chemistry*, (2019) 70, 99-102 [[Link](#)]
 3. J. Kang, S. H. Noh, J. Hwang, **H. Chun**, H. Kim, B. Han*, "First-principles database driven computational neural network approach to the discovery of active ternary nanocatalysts for oxygen reduction reaction", *Physical Chemistry Chemical Physics*, (2018) 20, 24539-24544 (Front Cover) [[Link](#)]
 2. H. Jung, J. Kang, **H. Chun**, B. Han*, "First principles computational study on hydrolysis of hazardous chemicals phosphorus trichloride and oxychloride (PCl₃ and POCl₃) catalyzed by molecular water clusters", *Journal of Hazardous Materials*, (2018) 341, 457-463 [[Link](#)]
 1. C. Kwon, S. H. Noh, **H. Chun**, I. S. Hwang, B. Han*, "First principles computational studies of spontaneous reduction reaction of Eu (III) in eutectic LiCl-KCl molten salt", *International Journal of Energy Research*, (2018) 42, 2757-2765 (Front Cover) [[Link](#)]

PATENTS

3. **Korea** Patent App. 10-2023-0067511 - Patent Method for Predicting Potential Energy of Multicomponent Materials
2. **U.S.** Patent App. 17523372, **China** Patent App. 202111501346.6, **Korea** Patent App. 10-2021-0037961 - Method for Performing Molecular Design of Ternary Catalyst Using Machine Learning
1. **U.S.** Patent App. 17286106, **Korea** Patent No. 10-2018-0124342 - Method for Prediction of Absorbance Change by Intermolecular Interaction

PRESENTATIONS

17. Machine-learning Accelerated Investigation of Compositional and Configurational Space of Nanocatalysts,

ICSE2023, Busan, Korea (Nov. 2023), **Invited Talk**

16. Active Learning Exploration of Single Atom Active Sites for Oxygen Reduction and Evolution Reactions, *AIChE Annual Meeting*, Orlando, USA (Nov. 2023), **Oral presentation**
15. High-throughput Virtual Screening of Single Atom Catalysts for Oxygen Reduction and Evolution Reactions, *The Korean Institute of Surface Engineering*, Jeju Island, Korea (May 2023), **Oral presentation**
14. AI Accelerated Computational Design of Green Energy Materials, GEEF, Global Engagement & Empowerment Forum on Sustainable Development, Seoul, Korea (Feb. 2023) **Invited Talk**
13. Rational Design Strategy of Fe-M (M=3d metals) based Dual-atom Catalysts toward Oxygenate Reactions, *The Korean Institute of Surface Engineering*, Gwangju, Korea (Nov. 2022)
12. Active Learning Accelerated Atomic Level Local Environments Tuning of Single Atom Catalysts for Oxygenate Catalytic Reactions, *The Korean Institute of Chemical Engineers*, Busan, Korea (Oct. 2022), **Oral presentation**
11. Investigation into Structural Evolution of Single Nanoparticles during Thermal Treatment with Atomic Precision, *The Korean Institute of Surface Engineering*, Incheon, Korea (Jun. 2022)
10. Understanding Structure-Property Relation of Individual Colloidal Nanoparticles with Thermal Treatment, *The Korean Institute of Chemical Engineers*, Jeju Island, Korea (April 2022)
9. Rational Design of PtFeCu Ternary Electrocatalyst for Oxygen Reduction Reaction, *The Korean Institute of Metals and Materials*, Jeju Island, Korea (Oct. 2021)
8. First-principles Study on the Role of Halogen Anion for Halospinel Solid-State Electrolyte, *MRS Korea*, Virtual, Korea (May 2021)
7. Machine-Learning Driven Potential Energy Surface for Nanoparticles Alloy System towards Oxygen Reduction Reaction, *AIChE Annual Meeting*, Virtual, USA (Nov. 2020)
6. First-Principles Computational Study of the Adsorption Mechanism for CH₃I(g) Removal, *AIChE Annual Meeting*, Orlando, USA (Nov. 2019), **Oral presentation**
5. Highly Efficient Adsorbents for Removal of Gaseous Methyl Iodide Using Tertiary Amines Impregnated Activated Carbon, *NANO KOREA 2019*, Ilsan, Korea (July 2019)
4. 아민 침착 활성탄에서의 유기요오드 흡착 제거능 평가 및 메커니즘 분석, Korean Institute of Hazardous Materials, Busan, Korea (July 2019), **Oral presentation**
3. 제일원리 전산모사를 통한 침착활성탄의 유기요오드 흡착능 평가, I/AMSEC, Daejeon, Korea (Nov. 2018), **Oral presentation**
2. First-Principles Computational Study of the Adsorption Mechanism of CH₃I(g) on Activated Carbon and Transition Metal Surfaces, *8th Pacific Basin Conference on Adsorption Science and Technology*, Sapporo, Japan (Sep. 2018), **Oral presentation**
1. First principles computational study on the adsorption mechanism of organic methyl iodide gas on triethylenediamine impregnated activated carbon, *2016 AIChE Annual Meeting*, San Francisco, USA (Nov. 2016)