

## Curriculum Vitae

# HOJE CHUN

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## RESEARCH/PROFESSIONAL EXPERIENCES

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<b>Postdoctoral Researcher</b> ( <i>Advisor</i> : Prof. Byungchan Han) Department of Chemical and Biomolecular Engineering Yonsei University, Seoul, Korea	<i>Mar. 2023</i> ~ <i>Present</i>
<b>Visiting Graduate Student Researcher</b> ( <i>Advisor</i> : Prof. Rafael Gomez-Bombarelli) Department of Materials Science and Engineering, <b>Massachusetts Institute of Technology</b> , Boston, USA	<i>July 2022</i> ~ <i>Sep. 2022</i>

## EDUCATION

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

## RESEARCH INTERESTS

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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

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<b>Global Ph.D. Fellowship, The National Research Foundation of Korea (NRF)</b>	<i>2019-2023</i>
Best Poster Award, The Korean Institute of Surface Engineering	<i>24 June 2022</i>
Best Poster Award, The Korean Institute of Chemical Engineers	<i>28 Oct. 2022</i>
Best Poster Award, The Korean Institute of Metals and Materials	<i>21 Nov. 2021</i>
BK21 Graduate Student Award, Yonsei University	<i>04 Feb. 2021</i>
Best Poster Award (Gold Medal), Nano Korea 2019	<i>05 July 2019</i>

## PUBLICATIONS (Total publications: 33 | First author publications: 15)

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+ = Equal contribution, \* = Corresponding author

### First author papers:

15. **H. Chun**<sup>+</sup>, J. Kang<sup>+</sup>, D. Kang, S. J. Hong, J. Heo, B. H. Kim<sup>\*</sup>, J. Park<sup>\*</sup>, B. Han<sup>\*</sup>, “Structural dynamics

and individual site catalytic activity of ligand protected platinum nanoparticles”, In preparation

14. D. G. Park<sup>+</sup>, J. W. Choi<sup>+</sup>, **H. Chun<sup>+</sup>**, H. S. Jang, H. Lee, W. H. Choi, B. C. Moon, K-H. Kim, M. G. Kim, B. Han<sup>\*</sup>, K. M. Choi<sup>\*</sup>, and J. K. Kang<sup>\*</sup>, “Increasing CO binding energy and defects by preserving Cu oxidation state via O<sub>2</sub> plasma-assisted N doping on CuO enables high C<sub>2</sub><sup>+</sup> selectivity and long-term stability in electrochemical CO<sub>2</sub> reduction”, *ACS Catalysis*, In revision
13. J. Lee<sup>+</sup>, X. A. Le<sup>+</sup>, **H. Chun<sup>+</sup>**, T. H. Vu, D. Choi, B. Han<sup>\*</sup>, M. I. Kim<sup>\*</sup>, and J. Lee<sup>\*</sup>, Active site engineering of Zn-doped mesoporous ceria toward highly efficient organophosphorus hydrolase-mimicking nanozyme, *Advanced Science*, In Revision
12. S. Hyun<sup>+</sup>, **H. Chun<sup>+</sup>**, M. Hong, J. Kang, and B. Han<sup>\*</sup>, First-principles Study on Ultrafast Li-ion Diffusion in Halospinel Li<sub>2</sub>Sc<sub>2/3</sub>Cl<sub>4</sub> through Multichannel Designed by Aliovalent Dopants, *Journal of Materials Chemistry A*, (2023) 11, 8, 4272-4279 [[Link](#)]
11. S. W. Koh<sup>+</sup>, J. Hu<sup>+</sup>, **H. Chun<sup>+</sup>**, P. Yu<sup>+</sup>, J. Ge, Z. Sun, W. Hong, Q. Liu, K. Nam, B. Han<sup>\*</sup>, Z. Liu<sup>\*</sup>, H. Li<sup>\*</sup>, “Two-dimensional palladium phosphonitride for enhanced oxygen reduction reaction”, *Applied Materials & Interfaces*, (2022)14, 10, 12156-12167 [[Link](#)]
10. D. K. Yesudoss<sup>+</sup>, **H. Chun<sup>+</sup>**, B. Han<sup>\*</sup>, S. Shanmugam<sup>\*</sup>, “Accelerated N<sub>2</sub> reduction kinetics via Synergistic Charge Transfer in Hybrid NbTiO<sub>4</sub> electrocatalyst”, *Applied Catalysis B: Environmental*, (2021) 304, 120938 [[Link](#)]
9. **H. Chun<sup>+</sup>**, E. Lee<sup>+</sup>, K. Nam, JH. Jang, W. Kyoung, S. H. Noh<sup>\*</sup>, B. Han<sup>\*</sup>, “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<sup>+</sup>, **H. Chun<sup>+</sup>**, J. Lee, BH. Kim, M. H. Seo, J. Kang<sup>\*</sup>, B. Han<sup>\*</sup>, “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<sup>+</sup>**, K. Nam, S. J. Hong, J. Kang<sup>\*</sup>, B. Han<sup>\*</sup>, “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<sup>+</sup>**, D. Choi<sup>+</sup>, J. Kang, J. S. Park, B. Han<sup>\*</sup>, "First-principles computational study of Ni/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub> hybrid interface reactions under extreme thermodynamic conditions", *Applied Surface Science*, (2020) 509, 144861 [[Link](#)]
5. K. Nam<sup>+</sup>, **H. Chun<sup>+</sup>**, J. Hwang, B. Han<sup>\*</sup>, "First-principles design of highly functional sulfide electrolyte of Li<sub>10-x</sub>SnP<sub>2</sub>S<sub>12-x</sub>Cl<sub>x</sub> for all solid-State Li-ion battery applications", *ACS Sustainable Chemistry & Engineering*, (2020) 8, 8, 3321-3327 [[Link](#)]
4. GY. Cha<sup>+</sup>, **H. Chun<sup>+</sup>**, DY. Hong<sup>+</sup>, J. Kim, KH. Cho, UH. Lee, JS. Chang, S. G. Ryu<sup>\*</sup>, H. W. Lee, SJ. Kim<sup>\*</sup>, B. Han<sup>\*</sup>, Y. K. Hwang<sup>\*</sup>, "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<sup>+</sup>, **H. Chun<sup>+</sup>**, H. C. Lee, Y. Lee, S. Lee, H. Jung, B. Han<sup>\*</sup>, 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<sup>\*</sup>, "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<sup>\*</sup>, "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:

18. J. Heo<sup>+</sup>, D. Kim<sup>+</sup>, H. Choi<sup>+</sup>, S. Kim, **H. Chun**, C. F. Reboul, C. T. S. Van, D. Elmlund, S. Choi, K. Kim, Y. Park, H. Elmlund<sup>\*</sup>, B. Han<sup>\*</sup>, and J. Park<sup>\*</sup>, "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<sup>\*</sup>, B. Han<sup>\*</sup>, L. YS. Lee<sup>\*</sup>, 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<sup>\*</sup>, "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<sup>+</sup>, D. Kim<sup>+</sup>, S. J. Hong<sup>+</sup>, X. Zhang, H. Hong, **H. Chun**, B. Han<sup>\*</sup>, L. YS. Lee<sup>\*</sup>, Y. Piao<sup>\*</sup>, 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<sup>\*</sup>, B. H. Kim<sup>\*</sup>, Jungwon Park<sup>\*</sup>, "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<sup>\*</sup>, Outstanding Stability of Gd-doped UO<sub>2</sub> 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<sup>+</sup>, JM. Lee<sup>+</sup>, **H. Chun**, Y. Lee, S. J. Hong, H. Jung, YJ. Kim, WG. Kim, V. Devaraj, E. J. Choi, JW. Oh<sup>\*</sup>, B. Han<sup>\*</sup>, "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<sup>+</sup>, J. W. Choi<sup>+</sup>, I. Jeon<sup>+</sup>, 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<sup>\*</sup>, M. Song<sup>\*</sup>, JW. Oh<sup>\*</sup>, Chuanbin Mao<sup>\*</sup>, "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<sup>\*</sup>, "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<sup>\*</sup>, "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<sup>\*</sup>, "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<sup>+</sup>, J. Heo<sup>+</sup>, 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<sup>\*</sup>, H. Elmlund<sup>\*</sup>, J. Park<sup>\*</sup>, "Critical differences in 3D atomic structure of individual ligand-protected nanocrystals in solution", *Science*, (2020) 368, 60-67 (Front Cover) [[Link](#)]
5. Y. Zhao<sup>+</sup>, J. Hwang<sup>+</sup>, M. T. Tang, **H. Chun**, X. Wang, H. Zhao, K. Chan, B. Han<sup>\*</sup>, P. Gao<sup>\*</sup>, H. Li<sup>\*</sup>, "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<sup>\*</sup>, "Elucidation of hydrolysis reaction mechanism of tungsten hexafluoride (WF<sub>6</sub>) 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 ( $\text{PCl}_3$  and  $\text{POCl}_3$ ) 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

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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

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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)
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  $\text{CH}_3\text{I(g)}$  Removal, *AIChE Annual Meeting*, Orlando, USA (Nov. 2019)
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)
3. 제일원리 전산모사를 통한 침착활성탄의 유기요오드 흡착능 평가, I/AMSEC, Daejeon, Korea (Nov. 2018)

2. First-Principles Computational Study of the Adsorption Mechanism of  $\text{CH}_3\text{I}(\text{g})$  on Activated Carbon and Transition Metal Surfaces, *8<sup>th</sup> Pacific Basin Conference on Adsorption Science and Technology*, Sapporo, Japan (Sep. 2018)
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)