

Hoje Chun

Integrated M.S. & Ph.D

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POSITIONS

<i>Mar. 2018 ~</i>	Yonsei University	Seoul, Korea
<i>Present</i>	Department of Chemical and Biomolecular Engineering Ph. D. Student <i>Advisor: Byungchan Han</i>	
<i>June. 2016 ~</i>	Yonsei University	Seoul, Korea
<i>Feb. 2018</i>	Department of Chemical and Biomolecular Engineering Research Internship, HANS Lab	

EDUCATION

<i>Mar. 2014 ~</i>	Yonsei University	Seoul, Korea
<i>Feb. 2018</i>	Department of Energy and Environmental Science and Engineering B.S. in Energy and Environmental Science and Engineering	

RESEARCH INTERESTS

Machine-Learning Atomic Potential & Computational Platform

Nanomaterials: Investigation of nanoparticles dynamics and their functionalities

Sustainable & Energy Materials: First-principles calculations of functional materials

HONORS & AWARDS

<i>2019-Present</i>	Global Ph.D. Fellowship, The National Research Foundation of Korea (NRF)
<i>04 Feb. 2021</i>	BK21 Graduate Student Award
<i>05 July 2019</i>	Best Poster Award (Gold Medal), Nano Korea 2019

PUBLICATIONS

(+ = Co-first Author, * = Corresponding Author, Total Publications = 16, Publications as a First Author = 6)

1. Jong-Min Lee, Jin Woo Choi, Il Jeon, Ye Zhu, Tao Yang, **Hoje Chun**, Jongmoon Shin, Juyun Park, Joohee Band, Kyounga Lim, Won-Geun Kim, Yeji Kim, Hyuk Jeong, Eun Jung Choi, Vasanthan Devaraj, Jeong Seok Nam, Hyungju Ahn, Yong-Cheol Kang, Byungchan Han, Myungkwan Song, Jin-Woo Oh, Chuanbin Mao "High quantum efficiency and stability of biohybrid quantum dots nanojunctions in bacteriophage-constructed perovskite", MATERIALS TODAY NANO (2021)
2. Jungyun Park, Jong-Min Lee, **Hoje Chun**, Yujin Lee, Sung Jun Hong, Hyunwook Jung, Ye-Ji Kim, Won-

- Geun Kim, Vasanthan Devaraj, Eun Jung Choi, Jin-Woo Oh, Byungchan 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)
3. Ga-Young Cha+, **Hoje Chun**+, Do-Young Hong+, Jaegyem Kim, Kyung-Ho Cho, U-Hwang Lee, Jong-San Chang, Sam Gon Ryu, Hae Wan Lee, Seung-Joo Kim, Byungchan Han, Young Kyu 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)
 4. Sung Jun Hong, **Hoje Chun**, Kyung Ah Min, Byungchan Han, "First-principles mechanism study on distinct optoelectronic properties of Cl-doped 2D hybrid tin iodide perovskite", *JOURNAL OF MATERIALS CHEMISTRY C*, (2020)
 5. Kyungju Nam, **Hoje Chun**, Jeemin Hwang, Kyung Ah Min, Byungchan Han, "Pairing of Transition Metal Dichalcogenides and Doped Graphene for Catalytically Dual Active Interfaces for the Hydrogen Evolution Reaction", *ACS SUSTAINABLE CHEMISTRY & ENGINEERING*, (2020)
 6. Yunxing Zhao, Jeemin Hwang, Michael T. Tang, **Hoje Chun**, Xingli Wang, Hu Zhao, Karen Chan, Byungchan Han, Pingqi Gao, Hong Li, "Ultrastable molybdenum disulfide-based electrocatalyst for hydrogen evolution in acidic media", *JOURNAL OF POWER SOURCES*, (2020)
 7. Byung Hyo Kim, Junyoung Heo, Sungin Kim, Cyril F. Reboul, **Hoje Chun**, Dohun Kang, Hyeonhu Bae, Hyejeong Hyun, Jongwoo Lim, Hoonkyung Lee, Byungchan Han, Taeghwan Hyeon, A. Paul Alivisatos, Peter Ercius, Hans Elmlund, Jungwon Park, "Critical differences in 3D atomic structure of individual ligand-protected nanocrystals in solution", *SCIENCE*, (2020)
 8. **Hoje Chun**+, Daehyeon Choi+, Joonhee Kang, Jung Su Park, Byungchan Han, "First-principles computational study of Ni/ α -Al₂O₃ hybrid interface reactions under extreme thermodynamic conditions", *APPLIED SURFACE SCIENCE*, (2020)
 9. Kyungju Nam+, **Hoje Chun**+, Jeemin Hwang, Byungchan Han, "First-Principles Design of Highly Functional Sulfide Electrolyte of Li₁₀-xSnP₂S₁₂- xCl_x for All Solid-State Li-Ion Battery Applications", *ACS SUSTAINABLE CHEMISTRY & ENGINEERING*, (2020)
 10. Keon Ho+, **Hoje Chun**+, Hyung Chae Lee, Yunjo Lee, Seulah Lee, Hyunwook Jung, Byungchan Han, Chang-Ha 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)
 11. Hyunwook Jung, Jeemin Hwang, **Hoje Chun**, Byungchan Han, "Elucidation of hydrolysis reaction mechanism of tungsten hexafluoride (WF₆) using first-principles calculations", *JOURNAL OF INDUSTRIAL AND ENGINEERING CHEMISTRY*, (2019)
 12. Joonhee Kang, Seung Hyo Noh, Jeemin Hwang, **Hoje Chun**, Hansung Kim, Byungchan 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)
 13. Choah Kwon, Seung Hyo Noh, **Hoje Chun**, Il Soon Hwang, Byungchan Han, "First principles computational studies of spontaneous reduction reaction of Eu(III) in eutectic LiCl-KCl molten salt", *INTERNATIONAL JOURNAL OF ENERGY RESEARCH*, (2018)
 14. **Hoje Chun**, Joonhee Kang, Byungchan 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)
 15. Hyunwook Jung, Joonhee Kang, **Hoje Chun**, Byungchan Han, "First principles computational study on hydrolysis of hazardous chemicals phosphorus trichloride and oxychloride (PC₃ and POCl₃) catalyzed

by molecular water clusters", JOURNAL OF HAZARDOUS MATERIALS, (2018)

16. **Hoje Chun**, Joonhee Kang, Byungchan Han, "First principles computational study on the adsorption mechanism of organic methyl iodide gas on triethylenediamine impregnated activated carbon", PHYSICAL CHEMISTRY CHEMICAL PHYSICS, (2016)

PATENTS

1. Method for Prediction of Absorbance Change by Intermolecular Interaction, International (PCT), (Oct. 2018)
2. 분자 간 상호작용에 의한 흡광도 변화 예측 방법, 10-2018-0124342 (Oct. 2018)

PRESENTATIONS

1. Machine-Learning Driven Potential Energy Surface for Nanoparticles Alloy System towards Oxygen Reduction Reaction, Virtual, USA (Nov. 2020)
2. First-Principles Computational Study of the Adsorption Mechanism for CH₃I(g) Removal, AIChE, Orlando, USA (Nov. 2019)
3. 아민 침착 활성탄에서의 유기요오드 흡착 제거능 평가 및 메커니즘 분석, Korea Institute of Hazardous Materials, Busan, Korea (July 2019)
4. Highly Efficient Adsorbents for Removal of Gaseous Methyl Iodide Using Tertiary Amines Impregnated Activated Carbon, NANO KOREA 2019, Ilsan, Korea (July 2019)
5. 제일원리 전산모사를 통한 침착활성탄의 유기요오드 흡착능 평가, 11th International Army Modeling & Simulation Education Conference, Daejeon, Korea, (Nov. 2018)
6. 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)
7. 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)