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Pohang University of Science and Technology (POSTECH) Researcher
Postage Project: Development of Kinetic Monte Carlo (KMC) simulation tool for the

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Research Project: Development of Kinetic Monte Carlo (KMC) simulation tool for the analysis of molecular-level of thin film deposition process

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• 2017	Kyeounghak Kim [†] , JeongDo Yoo [†] , Siwon Lee, Minseok Bae, Joongmyeon Bae, WooChul Jung [*] , and Jeong Woo Han [*] , A Simple Descriptor to Rapidly Screen CO Oxidation Activity on Rare-Earth Metal Doped CeO ₂ : from Experiment to First-Principles, ACS Appl. Mater. Interfaces 9 (2017) 15449-15458. †co-first authors (IF=7.504)
• 2017	Shin Wook Kang, <u>Kveounghak Kim</u> , Dong Hyun Chun, Jung-Il Yang, Ho-Tae Lee, Heon Jung, Jung Tae Lim, Sanha Jang, Chul Sung Kim, Chan-Woo Lee, Sang Hoon Joo*, Jeong Woo Han*, and Ji Chan Park*, High-performance $Fe_5C_2@CMK-3$ nanocatalyst for selective and high-yield production of gasoline-range hydrocarbons, J. Catal. 349 (2017) 66-74. (IF=6.844)
• 2017	<u>Kveounghak Kim</u> and Jeong Woo Han*, Mechanistic study for enhanced CO oxidation activity on (Mn,Fe) co-doped CeO ₂ (111), Catal. Today 293-294 (2017) 82-88. (IF=4.636)
• 2016	Kyeounghak Kim and Jeong Woo Han*, Effect of caffeic acid adsorption in controlling the morphology of gold nanoparticles: role of surface coverage and functional groups, Phys. Chem. Chem. Phys. 18 (2016) 27775-27783. (IF=4.449) *Selected as an Inside Back Cover
• 2016	Song-Hyun Cha, Youmie Park, Jeong Woo Han, <u>Kyeounghak Kim</u> , Hyun-Seok Kim, Hong-Lae Jang, and Seonho Cho*, Cold welding of gold nanoparticles on mica substrate: Self-adjustment and enhanced diffusion, Sci. Rep. 6 (2016) 32951. (IF=5.228)
• 2016	Hyun-Seok Kim, Yu Seon Seo, <u>Kyeounghak Kim</u> , Jeong Woo Han, Youmie Park, and Seonho Cho, Concentration Effect of Reducing Agents on Green Synthesis of Gold Nanoparticles: Size, Morphology, and Growth Mechanism, Nanoscale Res. Lett. 11 (2016) 1-9. (IF=2.584)
• 2016	Yeongdong Mun, Jongmin Shim, <u>Kveounghak Kim</u> , Jeong Woo Han, Soo-Kil Kim, Youngjin Ye, Jongkook Hwang, Seonggyu Lee, JongHyun Jang, Yong-Tae Kim, and Jinwoo Lee, Direct access to aggregation-free and small intermetallic nanoparticles in ordered, large-pore mesoporous carbon for electrocatalyst, RSC Adv. 6 (2016) 88255- 88264. (IF=3.289)
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• 2016	<u>Kyeounghak Kim</u> , Wonyoung Lee*, and Jeong Woo Han*, First-Principles Study of Enhanced Oxygen Incorporation near the Grain Boundary on Yttria-Stabilized Zirconia, Sci. Adv. Mater. 8 (2016) 196-200. (IF=1.812)
• 2015	Geonyeop Lee, Jihyun Kim*, <u>Kyeounghak Kim</u> , and Jeong Woo Han*, Precise control of defects in graphene by using oxygen plasma, J. Vac. Sci. Tech. A 33 (2015) 060602. *Featured as the MOST READ list this month (IF=1.464)
• 2015	Gwangseok Yang, Byung-Jae Kim, <u>Kyeounghak Kim</u> , and Jeong Woo Han*, and Jihyun Kim*, Energy and dose dependence of proton-irradiation damage in monolayer graphene, RSC Adv. 5 (2015) 31861-31865. (IF=3.840)
• 2013	Jeonghyun Ko [†] , Ho Seong Song [†] , <u>Kyeounghak Kim</u> [†] , and Jeong Woo Han *, Recent research trend in catalyst design based on density functional theory calculations, Catalysis 29 (2013) 1-16. [†] co-first authors

Selected Presentations

• 2023	<u>Kyeounghak Kim*</u> Computational design of energy materials, THE 1 st INTERNATIONAL CONFERENCE ON THE PRACTICAL ZERO EMISSIONS TECHNOLOGIES AND STRATEGIES (PZETS 2023), Ho Chi Minh City, Vietnam, Dec. 10, 2023. (invited talk)
• 2023	<u>Kyeounghak Kim*</u> Engineering of B-metal exsolution to design perovskite-based catalytic materials for efficient hydrogen production, KIChE Spring Meeting, Pusan, Korea, Apr. 21, 2023 (invited talk)
• 2023	<u>Kyeounghak Kim*</u> Computational design of exsolution catalysts for electrochemical reactions, KCERS Spring Meeting, Jeju, Korea, Apr. 12, 2023. (invited talk)
• 2022	Kyeounghak Kim* Engineering of cation stability for the design of perovskite-based electrode materials in solid oxide fuel cells, KIEC Fall Meeting, Daejeon, Korea, Nov. 2-4, 2022. * Miwon young researcher award (invited talk)
• 2022	Kyeounghak Kim*, Computational Design of Electrode Materials in Solid Oxide Fuel Cells: From fundamental to practical applications, KIEC Fall Meeting, Daejeon, Korea, Nov. 2-4, 2022. (JPI-KSIEC joint symposium) (invited talk)
• 2022	Kyeounghak Kim*, Computational Materials Design for Solid Oxide Fuel Cells, BK Seminar, Sungkyunkwan University, Suwon, Korea, Sep. 16, 2022. (<i>invited talk</i>)
• 2022	<u>Kyeounghak Kim*</u> , Computational Design of Electrode Materials in Solid Oxide Fuel Cells, BK Seminar, Yonsei University, Seoul, Korea, Aug. 5, 2022. (<i>invited talk</i>)
• 2022	Kyeounghak Kim*, Computational Design of Catalytic Materials for Hydrogen Production, Storage, and Applications, KIEC Spring Meeting, Jeju, Korea, May 11-13, 2022. (<i>invited talk</i>)
• 2022	Kyeounghak Kim*, Mechanistic Study of Hydrogen Production and Applications, KIEC Spring Meeting, Jeju, Korea, May 11-13, 2022. (<i>invited talk</i>)
• 2022	Kyeounghak Kim*, Basics of DFT calculation (technical training session), KIEC Spring Meeting, Jeju, Korea, May 11-13, 2022. (<i>invited talk</i>)
• 2022	Kyeounghak Kim*, Computational Materials Design for Energy Applications, KIChE Spring Meeting, Jeju, Korea, Apr. 20-23, 2022. (<i>invited talk</i>)
• 2022	<u>Kyeounghak Kim*</u> , Computational Design of Catalytic Materials, Nano-Convergence Technology Division, National Nanofab Center, Daejeon, Apr. 13, 2022. (<i>invited talk</i>)
• 2022	<u>Kyeounghak Kim*</u> , Computational Design of Electrode Materials in Solid Oxide Fuel Cells, KECS Spring Meeting, Jeju, Apr. 7, 2022. (<i>invited talk</i>)
rriculum vitae of	For more information go to

• 2022	Kyeounghak Kim* , Computational Design of Anode Materials in SOFCs, ERICA (Hanyang University) Department Seminar, Ansan, Mar. 10, 2022. (<i>invited talk</i>)
• 2022	Kveounghak Kim*, Engineering of B-metal Exsolution for Enhanced Anode Materials in Solid Oxide Fuel Cells, Nano Convergence 2022, Konjiam Resort, Jan. 19, 2022. (<i>invited talk</i>)
• 2021	Kyeounghak Kim*, Computational Chemistry in Chemical Engineering, Hanyang University, Seoul, Korea, May, 20, 2021. (<i>invited talk</i>)
• 2020	Kyeounghak Kim* , and Jeong Woo Han, Engineering of cation stability for highly stable and active perovskite-based SOFC electrode materials, KIChE Fall Meeting, Online, August 14-16, 2020. (<i>Best poster award</i>)
• 2019	Kyeounghak Kim* and Jeong Woo Han, "A DFT Study for Engineering of B-metal Exsolution Tendency in Perovskite Materials", KCS Fall Meeting, Seoul, Korea, November 13-15, 2019. (<i>oral presentation</i>)
• 2019	<u>Kveounghak Kim</u> [*] and Jeong Woo Han, Enhanced Catalytic Activity of CO Oxidation on Exsolved Co Nanoparticles by Controlling the Stability of B-metal (Co) in $SrTi_{1-x}Co_xO_{3-\delta}$, Korean SOFC symposium, Pusan, Korea, January 18-19, 2019. (<i>Best poster award</i>)
• 2018	<u>Kyeounghak Kim</u> [*] , and Jeong Woo Han, Controlling the Stability of B-metal (Co) in $SrTi_{1-x}Co_xO_{3-\delta}$ for Enhancing the Exsolution on Perovskite Materials, ENGE 2018, Jeju, Korea, Nov 11-14, 2018. (<i>Best poster award, Gold prize</i>)
• 2018	<u>Kyeounghak Kim</u> *, and Jeong Woo Han, How to Control B-metal Exsolution on Perovskite Materials, Materials Challenges in Alternative and Renewable Energy (MCARE), Vancouver, Canada, August 18-25, 2018. (<i>invited talk</i>)
• 2018	Kyeounghak Kim*and Jeong Woo Han, "Mechanistic Study for the Formation of Exsolved Alloy Nanoparticles on Transition Metal Doped PaBaMnO5+ δ under Reducing Environment", KIChE Spring Meeting, Daejeon, Korea, April 25-27, 2018. (oral presentation)(Best Research Presentation Award)
• 2017	Kyeounghak Kim* , Jinho Oh, Tae Wan Kim, Ji Hoon Park, Young-Woong Suh, and Jeong Woo Han, "Mechanistic Study of Catalytic Dehydrogenation of Decalin to Tetralin to Naphthalene on Pd(111) and Pt(111)" KIChE Spring Meeting, JeJu, Korea, April 26-28, 2017. (<i>oral presentation</i>) <i>*Hoimyung Research Award</i>
• 2016	Kyeounghak Kim and Jeong Woo Han*, "Density Functional Theory based Computational Screening of Metallic Nanoparticle Exsolution on ABB'O ₃ Perovskites", The International Conference on Technological Advances of Thin Films & Surface Coatings, Singapore, July 12-15, 2016 (<i>invited talk</i>)
• 2015	Kyeounghak Kim [*] and Jeong Woo Han, "Fast screening of CO oxidation activity on rare-earth metal doped CeO ₂ (111) surfaces", ICAE 2015, Jeju, Korea, November 17-20, 2015. (<i>Best poster award</i>)
• 2015	Kyeounghak Kim [*] , Wonyoung Lee, and Jeong Woo Han, "Density Functional Theory Study of Surface Oxygen Incorporation Mechanism on the Yttria-Stabilized Zirconia", Nano Korea, Seoul, Korea, July 1-3, 2015. (<i>Best poster award</i>)
• 2014	Kyeounghak Kim *, Wonyoung Lee, and Jeong Woo Han, "Mechanistic Studies of Enhanced Oxygen Incorporation near the Grain Boundary on Yttria-Stabilized Zirconia", The Korean Society of Clean Technology, Gyeongju, Korea, September 24-26, 2014. (<i>Best poster award</i>)

RESEARCH EXPERIENCES

• July 2024 – Present To Dec 2028 Co-Principal investigator (Co-PI)	"Development of Low-Cost Catalytic Materials for Distributed Ammonia Production and Utilization Based on Interface Engineering", National Research Foundation of Korea (NRF). <u>Co-Principal investigator, #100,000,000/year</u>
• July 2024 – Present To Dec 2028 Co-Principal investigator (Co-PI)	"Establishment of a HUB for Proton Conductive Materials for Water Electrolysis with Artificial Intelligence and Data", National Research Foundation of Korea (NRF). <u>Co-Principal investigator, #150,000,000/year</u>
• 2024 – Present To Dec 2028 <u>Core-Researcher</u>	"Establishment of CPU and GPU-based simulation clusters for surface and interface analysis", Infrastructure advancement project, Ministry of Education. <i>Core-Researcher</i> , #380,000,000
• Oct 2023 – Present To Sep 2024 Principal investigator (PI)	"Development of highly active catalyst for CO ₂ utilization", GS Caltex. <i>Principal investigator</i> , ₩70,000,000
• Apr 2024 – Dec 2024 Co-Principal investigator (Co-PI)	"Development of Exsolution Based Multi-Alloy Catalysts to Break the Inverse Relationship Between Activity and Durability", Engineering Research Center, National Research Foundation of Korea (NRF). <u>Co-Principal investigator</u> , <u>#10,000,000/year (Pre-planning)</u>
• July 2022 – Present To June 2029 Co-Principal investigator (Co-PI)	"Center for Decentralized Low-carbon Hydrogen Production", Engineering Research Center, National Research Foundation of Korea (NRF). <u>Co-Principal investigator</u> , <u>#120,000,000/year</u>
• Jun 2023 – Jun 2024 Principal investigator (PI)	"Elucidating the synthetic mechanism of Sulfide Solid Electrolytes via computational modeling and DFT calculations", SK On. <u><i>Principal investigator (PI), #70,000,000/year</i></u>
• Mar 2021 – Feb 2024 Principal investigator (PI)	"Controlling Cation Stability in Perovskite Based Electrode Materials for High Performance Solid Oxide Fuel Cells", Sejong Science Fellowship, National Research Foundation of Korea (NRF). <i>Principal investigator (PI)</i> , #135,000,000/year
• July 2022 – Dec 2023 Researcher	"Development of technology for the production of 100% biomass-based bioplasticizers replacing petroleum-based plasticizers. Climate Change Technology Development, National Research Foundation of Korea (NRF). <u>Researcher</u> , <u>#/30,000,000/year</u>
• Sep 2021 – Aug 2022 Principal investigator (PI)	"Computational design of catalyst for hydrogen production", Research funding for faculty member, Hanyang University. <u><i>Principal investigator</i>, #20,000,000/year</u>
• May 2021 – Apr 2022 Principal investigator (PI)	"Design of highly active and stable electrodes by controlling cation stability in perovskite based materials", KISTI HPC supercomputing resources support.
• Mar 2019 – Feb 2021 Principal investigator (PI)	"The development of enhance anode materials in SOFCs by using B-metal exsolution", Global PhD Fellowship, National Research Foundation of Korea (NRF). <u>Principal investigator (PI)</u> , #30,000,000/year
• Dec 2015 – Dec 2020 Main Researcher	"Research on technology and commercialization of metal-supported solid oxide fuel cell for utilization of hydrocarbon fuels", Korea Institute of Energy Technology Evaluation and Planning (KIETEP).
Page 10 - Curriculum vitae of [Kyeounghak Kim]	For more information go to http://ccel.postech.ac.kr/

• Dec 2016 – Dec 2020 Main Researcher	"In-situ growth of self-assembled metal nano-catalysts using spontaneous metal/oxide phase separation", Samsung Research Funding Center for Future Technology.
• Jan 2016 – Sep 2020 Main Researcher	"The multiscale technology for long-term stabilized SOFC", Global Frontier Center for Multiscale Energy System from the National Research Foundation of Korea.
• May 2016 – Mar 2019 Main Researcher	"Development of Liquid Organic Hydrogen Carriers as a Renewable Storage and Transport using Modified Heat-transfer Fluids", Korea Institute of Energy Technology Evaluation and Planning
• Feb 2018 – Feb 2019 Main Researcher	"Development of Kinetic Monte Carlo (KMC) simulation tool for the analysis of molecular-level of thin film deposition process", SK hynix, Inc.
• Dec 2015 – Aug 2018 Main Researcher	"Super Ultra Low Energy & Emission Vehicle Center", Engineering Research Center (ERC) from the National Research Foundation of Korea.
• May 2016 – Jan 2018 Main Researcher	"Development of single-atom electrocatalysts for H ₂ production and utilization", Samsung Research Funding Center for Future Technology
• Mar 2015 – Jas 2016 Main Researcher	"Rational design of key materials for high performance solid oxide and proton exchange membrane fuel cells via computational materials science", Global Frontier Center for Multiscale Energy System from the National Research Foundation of Korea
• May 2015 – Jan 2016 Main Researcher	"Green Synthesis of Gold Nanoparticles using Caffeic Acid (CA)", National Creative Research Initiatives Center for Isogeometric Optimal Design
• Oct 2015 – Aug 2016 Main Researcher	"Design of exsolved metal nano-catalysts using spontaneous metal/oxide phase separation for Intelligence electrode materials of SOFCs", KISTI HPC supercomputing resources support, (KSC-2015-C3-045) "Super science 2017" issued by KISTI HPC supercomputing center.
• Oct 2014 – Sep 2015 Main Researcher	"Design of electrode and electrolyte materials for SOFCs with high efficiency and stability", KISTI HPC supercomputing resources support, (KSC-2014-C2-048)

SOCIAL EXPERIENCES

• Apr 2022 – Present	Korean Federation of Science and Technology Societies (KOFST) Future Generation Committee, Member
• Jul 2023 – Present	Center for Women in Science, Engineering, and Technology (WISET) Future Generation Committee, Member
• Mar 2023 – Present	Presidential Committee for National Cohesion Science and Technology Committee, Member
• Jan 2022 – Dec 2023	The Korean Society of Industrial and Engineering Chemistry Catalyst Division, General Manager
• Jan 2015 – Present	The Korean Institute of Chemical Engineers Catalyst Division, Member
Research Interests	Energy Materials Lithium-ion Cell / Fuel Cell (SOFC & PEMFC)
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 $Catalytic Materials \\Automotive Catalyst / Hydrogen Production & Storage / CO_x & NO_x conversion / CO_2 \\utilization / Single Atom Catalyst / Reforming of CH_4 / HER / ORR / OER \\$

Simulation Tool Developments Monte Carlo Simulation / Beyond DFT / Machine Learning

HONORS / AWARDS

• 2024	Young Catalyst Scientist Award The Korean Institute of Chemical Engineers, Catalyst Division
• 2023	Miwon Young Researcher Award Miwon Commercial Co., Ltd. & The Korean Society of Industrial and Engineering Chemistry
• 2022	S-Oil Best Thesis Award S-Oil & National Academy of Engineering of Korea
• 2021	Best Graduate Student in 2021 BK21, POSTECH
• 2021	Sejong Research Fellowship National Research Foundation of Korea
• 2021	Graduate <i>summa cum laude</i> (Ph.D.) Dept. of Chemical Engineering in POSTCH
• 2021	Brain Korea21 (BK21) Scholarship Program (2018 ~ 2020) Korean Ministry of Education
• 2020	Graduate Student Research Award (Catalysis) The Korean Institute of Chemical Engineers, Fall Meeting
• 2020	Best Paper Award The Korean Institute of Chemical Engineers, Fall Meeting
• 2020	Best Paper Award BK21, POSTECH
• 2020	The First Prize at Daelim Research Award (Catalysis/Materials) Daelim Industrial Co. Ltd.
• 2019	Best Paper Award BK21, POSTECH
• 2019	Silver Prize (2nd) at Samsung Electro-Mechanics Research Award Samsung Electro-Mechanics Co. Ltd.
• 2019	Global PhD Fellowship National Research Foundation of Korea
• 2019	Best Poster Award at Korean SOFC symposium 2019
• 2018	Best Poster Award at ENGE 2018
• 2018	Best Research Presentation Award
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	The Korean Institute of Chemical Engineers, Spring Meeting
• 2017	Outstanding Paper Award II University of Seoul
• 2017	Hoimyung Research Award Hoimyung Industrial Co. Ltd. & KIChE
• 2017	Outstanding Paper Award I University of Seoul
• 2016	Outstanding Paper Award I University of Seoul
• 2015	Best Poster Award 3 th International Conference on Advanced Electromaterials (ICAE 2015)
• 2015	Best Poster Award 13 th International Nanotech Symposium (Nano Korea 2015)
• 2014	Best Poster Award at Fall Meeting The Korean Society of Clean Technology
Journal Reviewer	Nature Communications (Nature publishing group)
	Korean Journal of Chemical Engineering (Springer)
	Molecular Catalysis (Elsevier)
	Applied Surface Science (Elsevier)
	Chemical Engineering Journal (Elsevier)
	Electrochem (MDPI)
	Catalysis (MDPI)
	Physical Chemistry Chemical Physics (RSC)