

Byung-Hyun Kim, Ph.D.

Professor

Department of Energy and Bio Sciences, Department of Applied Chemistry
College of Engineering Sciences
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Professional Experience

Professor

Sep. 2026 – present

Dept. of Energy and Bio Sciences / Dept. of Applied Chemistry, Hanyang University ERICA

Visiting Scholar (Host: Prof. Yusuke Yamauchi)

Jul. 2026 – Feb. 2027

Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Australia

Associate Professor

Sep. 2023 – Aug. 2026

Dept. of Energy and Bio Sciences / Dept. of Applied Chemistry, Hanyang University ERICA

Senior/Principal Research Scientist

Jul. 2017 – Aug. 2023

Computational Science & Engineering Laboratory, Korea Institute of Energy Research

Chief of Computational Science & Engineering Laboratory

Jan. 2022 – Jul. 2023

Computational Science & Engineering Laboratory, Korea Institute of Energy Research

Postdoctoral Researcher (PI: Prof. Kersti Hermansson)

Feb. 2016 – Jun. 2017

Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden

Senior Engineer

Mar. 2013 – Jan. 2016

CAE Team, Semiconductor R&D Center, Samsung Electronics Co., Ltd.

Research Assistant (PI: Dr. Kwang-Ryeol Lee)

Feb. 2008 – Feb. 2013

Computational Science Research Center, Korea Institute of Science & Technology

Education

Ph.D. (PI: Prof. Yong-Chae Chung, Dr. Kwang-Ryeol Lee)

Feb. 2013

Dept. of Materials Science & Engineering, Hanyang University

Computational Science Research Center, Korea Institute of Science & Technology

Dissertation: *Multiscale Simulation Study of Interfacial Properties on Low Dimensional Materials: CNTs and SiNWs*

M.S. (PI: Prof. Yong-Chae Chung)

Feb. 2009

Dept. of Materials Science & Engineering, Hanyang University

Thesis: *Atomic-level Investigation of Deposition Behavior and Surface Characteristic of Co-Cu Multilayer System: Molecular Dynamics*

B.S.

Feb. 2007

Dept. of Ceramic Engineering, Hanyang University

Expertise

- **Computational electrochemistry and catalysis:** reaction mechanisms and active-site analysis for various reactions
- **Electronic structure and surface/defect chemistry of energy materials**
- **Machine learning for materials:** machine learning interatomic potentials; active-learning and multi-objective optimization for catalyst screening; descriptor discovery (SISSO); LLM-assisted literature mining
- **Multiscale simulation:** density functional theory, density functional based tight binding, classical and reactive molecular dynamics, kinetic Monte Carlo
- **Research data infrastructure:** FAIR materials-data platforms, plugin and workflow design
- **Software and computing:** VASP, LAMMPS, Gaussian, Materials Studio, QuantumATK, LOBSTER, pymatgen/ASE, OVITO, VESTA; Python, C/C++, shell; operation of an in-house HPC cluster and national supercomputing resources

Research Interests

- **Computational design of electrocatalysts for green hydrogen:** alkaline and PEM water electrolysis, saline/seawater electrolysis, and nitrate reduction coupling wastewater treatment with ammonia synthesis
- **AI-accelerated materials discovery:** active learning, machine-learned potentials, and LLM-based literature mining toward closed-loop catalyst design
- **Interfacial chemistry of next-generation batteries:** zinc, sodium, and lithium metal anodes, host architectures, and electrolyte additives
- **Solar-driven chemical conversion:** photoelectrochemical water splitting, CO₂-to-fuel conversion, and biomass/lignin valorization
- **Surface chemistry for semiconductor manufacturing:** discovery of new corrosion inhibitors, and metal-ion and particle interactions in post-CMP cleaning
- **Research data ecosystems for materials science**

Journal Publications

- [76] **Chemistry of Selective Metal Ions Adsorption and Loading onto PVAc Polymer Brush during Advanced Metal Post-CMP Cleaning**
Maheepal Yadav, Sanjay Bisht, **Byung-Hyun Kim**, Se-Hoon Park, Tae-Gon Kim, Jihoon Seo*, and Jin-Goo Park*
Applied Surface Science 752, 168292 (2027) · IF 6.6, Top 19.1% (JCR 2025) · doi:10.1016/j.apsusc.2026.168292
- [75] **Redox-Active Ligand-Stabilized Lithium Iron Phosphate Nanoparticles for High-Performance Lithium-Ion Battery Cathode with High Capacities and Long-Term Stability**
Jiwon Bok†, Jeongyeon Ahn†, Bogeun Park†, Donghyeon Nam†, Hee Seung Ryu, Uijun Lee, Jaeyeong Jang, Shihyun Chang, Sungha Choi, Minseong Kwon, Woojae Chang, Du Yeol Ryu, Daegun Kim, Hee-Dae Lim, **Byung-Hyun Kim***, Yongmin Ko*, and Jinhan Cho*
Nano-Micro Letters 19, 12 (2027) · IF 38.5, Top 0.8% (JCR 2025) · doi:10.1007/s40820-026-02313-6
- [74] **Single-Atom Active Sites in Polymeric Phthalocyanine Hybrid Electrocatalysis for High-Efficiency Lithium–Carbon Dioxide Batteries**
Huiju Kim†, Jun Su Kim†, Hunchol Seo†, Yeji Lim, Suji Kim, Yoon Jeong Yoo, Yoonbin Kim, Won Il Kim, Hyun Chul Kim, Minhyeok Choi, Kihyun Shin, **Byung-Hyun Kim***, Ho Seok Park*, and Won-Hee Ryu*
Advanced Functional Materials e78821 (in press) · IF 19.9, Top 4.2% (JCR 2025) · doi:10.1002/adfm.78821
- [73] **Sustainable Low-Valent Iridium Active Sites in Rhenium Doped Perovskite Iridates for Efficient Acidic Oxygen Evolution Reaction via Hybridized Reaction Pathways**
SungJae Park†, Jaekyum Kim†, Daehee Yang†, Jinkyu Lim†, Seong Hyun Park, Min Gyu Choi, Kang Taek Lee, Jihye Lee, Ashishi Gaur, Ghulam Ali, Haryeon Baek, In-Hui Hwang, Mingony Kim, Kyung Yoon Chung, Jung Kyu Kim*, Young-Min Kim*, **Byung-Hyun Kim***, and HyukSu Han*
Angewandte Chemie-International Edition e1466065 (in press) · IF 17.6, Top 6.2% (JCR 2025) · doi:10.1002/anie.1466065

- [72] **Upcycled Polymer Waste-Derived N-Doped Carbon Supports Enabling Durable PtCo Catalysts for PEM Fuel Cells**
Yewon Kim†, Daehyeon Seo†, Min Seo Kim, Su Min Ahn, Se Youn Cho, Yunji Kim, Jiho Choi, **Byung-Hyun Kim***, Hongseok Yun*, and Young Jun Lee*
Chemical Engineering Journal 547, 180588 (2026) · IF 12.5, Top 4.0% (JCR 2025) · doi:10.1016/j.cej.2026.180588
- [71] **Synergistic Corrosion Inhibition of Interfacially Engineered Al-O/CNT Composites through Al-O-C Chemical Anchoring**
Seon-Min Kim, Seoyoon Gong, JaeBeom Hwang, **Byung-Hyun Kim**, Donghyun Bae, and Se-Eun Shin*
npj Materials Degradation 10, 121 (2026) · IF 7.5, Top 23.2% (JCR 2025) · doi:10.1038/s41529-026-00865-x
- [70] **Solar-thermal 3D-interconnected Macroporous Carbon Nanoreactors for Solvent-minimized Paste-state Suzuki Coupling**
Dongchan Lee†, Incheol Heo†, YongJoo Kim, **Byung-Hyun Kim**, Hyungphil Chun, Michael Tsapatsis, Won Cheol Yoo*, and Kwang-Suk Jang*
Chemical Engineering Journal 547, 179658 (2026) · IF 12.5, Top 4.0% (JCR 2025) · doi:10.1016/j.cej.2026.179658
- [69] **Diverting the Use of Reduced TiO₂ from a Carrier of Electron–Hole Pairs to a Reservoir of Brønsted–Lewis Acidic Pairs for Sustainable, Non-Optical H₂O₂ Homolysis**
Minsung Kim†, Gyuchan Kim†, Junseo Kim, Sang Hoon Kim*, **Byung-Hyun Kim***, and Jongsik Kim*
Journal of Materials Chemistry A 14, 28907 (2026) · [Inside Front Cover](#) · IF 9.2, Top 17.3% (JCR 2025) · doi:10.1039/D6TA01339B
- [68] **Breaking the Water Dissociation–Hydrogen Adsorption Trade-off through W Single-Atom Engineering for Alkaline Hydrogen Evolution**
Taeyoung Jeong†, Gyuchan Kim†, **Byung-Hyun Kim***, and Myeongjin Kim*
Applied Catalysis B: Environment and Energy 399, 127056 (2026) · IF 19.7, Top 1.7% (JCR 2025) · doi:10.1016/j.apcatb.2026.127056
- [67] **Facilitating Hydrogen Evolution Reaction Activity in Alkaline Water Electrolysis via Formation of Ni-Co₂P Heterojunction**
Junseok Sim†, Wan Sik Kim†, Jaekyum Kim, Asiya M. Tamboli, Younghan Jung, Sejin Im, JunSeok Oh, Jung Kyu Kim, **Byung-Hyun Kim***, and Chang-Hee Kim*
Energy & Environmental Materials e70385 (in press) · IF 13.8, Top 10.2% (JCR 2025) · doi:10.1002/eem2.70385
- [66] **Vacancy-Mediated Dual-Step Phosphorization–Sulfurization of MnMoO₄ for Efficient Acidic Hydrogen Evolution**
Jyoti Ganapati Badiger, Chae-Eun Lim, Fawad Tariq, Maheswari Arunachalam, Suzan Abdelfattah Sayed, Alaa M. Ibrahim, Sang-Wan Ryu, **Byung-Hyun Kim***, and Soon Hyung Kang*
Journal of Materials Chemistry A 14, 26673 (2026) · [Front Cover](#) · IF 9.2, Top 17.3% (JCR 2025) · doi:10.1039/D6TA01695B
- [65] **Active Learning-Driven Multi-Objective Design of High-Entropy Alloy Catalysts for Saline Water Electrolysis**
Kwangsoo Kim, Matthew J. Wolf, YongJoo Kim*, and **Byung-Hyun Kim***
Chemical Engineering Journal 536, 176134 (2026) · IF 12.5, Top 4.0% (JCR 2025) · doi:10.1016/j.cej.2026.176134
- [64] **Spatially Extended Interfacial Optimization via Holey-Defect Architectures for Hydrogen Evolution Reaction**
Chengang Pei†, Jaekyum Kim†, Dong Zhang, Won Tae Hong, Jong Hun Kim, Xu Yu, Jongwook Park, Chan-Hwa Chung, **Byung-Hyun Kim***, Ho Seok Park*, and Jung Kyu Kim*
Small 22, e00032 (2026) · IF 11.8, Top 8.1% (JCR 2025) · doi:10.1002/smll.202600032
- [63] **Molybdenum Ion-Induced Adhesion of Colloidal Silica to Polyvinyl Acetal Brushes in Post-Chemical Mechanical Planarization Applications: Experiments and Multiscale Simulations**
Sumit Kumar, Palwasha Jalalzai, Tae-Gon Kim, Jihoon Seo, Junsang Lee, Gayoung Kim, In-Kwon Kim, Sangkyun Kim, **Byung-Hyun Kim***, and Jin-Goo Park*
ACS Applied Materials & Interfaces 18, 27086 (2026) · IF 7.8, Top 22.4% (JCR 2025) · doi:10.1021/acsami.6c05073
- [62] **All-Inorganic Perovskite@SiO₂ Quantum Dots for Amplifying the Interfacial Electric Field on WO₃ Toward Enhanced Photoelectrochemical Water Splitting**
Won Tae Hong†, Yuankai Li†, Jaekyum Kim, Dokyum Kim, Jaemin Park, Woosok Yang, Jongwook Park, Hanleem Lee, Chang Hyuck Choi, **Byung-Hyun Kim**, Chang-Lyoul Lee*, Tae-Hoon Kim*, and Jung Kyu Kim*
SusMat 6, e70066 (2026) · IF 19.2, Top 2.2% (JCR 2025) · doi:10.1002/sus2.70066

- [61] **Electric-Field-Driven Bilayer Interphase from Oxygenated Nanodiamond-Carbon Nanoparticles for Dendrite-Free Lithium Metal Batteries**
Jaeseong Kim†, Incheol Heo†, Dong-Kyung Kim†, Min Seok Kang, Ji Hee Kwon, Byeong-Seon An, Keir C. Neuman, **Byung-Hyun Kim***, Hak-Sung Jung*, and Won Cheol Yoo*
Advanced Energy Materials 16, e05964 (2026) · IF 25.5, Top 2.4% (JCR 2025) · doi:10.1002/aenm.202505964
- [60] **Methane Diffusion Path in HKUST-1 Metal–Organic Framework Revealed by Atomistic Simulations**
Hyo-Sun Jang†*, Eunyeong Cho†, Gyuchan Kim, Hee Jung Lee, Jae-Hyung Cho, and **Byung-Hyun Kim**
Scientific Reports 16, 16413 (2026) · IF 4.9, Top 14.6% (JCR 2025) · doi:10.1038/s41598-026-45125-9
- [59] **Geometrically-Screened, Sterically-Hindered Additive for Wide-Temperature Aqueous Zinc-Ion Batteries**
Sida Zhang, Shengyang Huang, Weigen Chen*, Zuyang Hu, Dong Hyun Min, Jun Su Kim, Hao Fu, Young Soo Yun, Won-Chul Cho, **Byung-Hyun Kim**, Baoyu Li*, Chengchao Li, Jingyu Sun, and Ho Seok Park*
Advanced Functional Materials 36, e23753 (2026) · IF 19.9, Top 4.2% (JCR 2025) · doi:10.1002/adfm.202523753
- [58] **3D Channeled Porous Carbon Hosts with Cobalt Nanoparticle-Induced Zincophilicity for Stable Zinc Anodes**
Hyunsoo Lee†, Donghyeon Nam†, Chaehyeon Moon, Jinseok Park, Michael J. Lee, Keun Hee Kim, Hyeonsoo Han, Donghyeok Roh, Kyungmo Kim, Jaeyoung Choi, Seung Woo Lee, **Byung-Hyun Kim***, Young Jun Lee*, and Bumjoon J. Kim*
Chemical Engineering Journal 529, 172613 (2026) · IF 12.5, Top 4.0% (JCR 2025) · doi:10.1016/j.cej.2026.172613
- [57] **Cobalt Ion Adsorption on Polyvinyl Acetal Brushes: Impact on Silica-Nanoparticle Loading During Metal Post-Chemical Mechanical Planarization Cleaning**
Maheepal Yadav, Sanjay Bisht, **Byung-Hyun Kim**, Hirokuni Hiyama, Tae-Gon Kim, and Jin-Goo Park*
ACS Applied Nano Materials 9, 237 (2026) · IF 5.8, Top 31.2% (JCR 2025) · doi:10.1021/acsanm.5c04532
- [56] **Roles of Alkaline-Earth Metals and Electron Density of Al³⁺ in Octanol Dehydration for Linear Alpha-Olefin Production**
Young-eun Kim†, Jaekyum Kim†, Unho Jung, Yongha Park, Min Hye Youn, Dong Hyun Chun, Byeong-Seon An, Jung Kyu Kim, **Byung-Hyun Kim***, Ki Bong Lee*, and Kee Young Koo*
Journal of Materials Chemistry A 14, 403 (2026) · [Back Cover](#) · IF 9.2, Top 17.3% (JCR 2025) · doi:10.1039/D5TA06534H
- [55] **Molecularly Dispersed Polyoxometalate Clusters via Polymeric Ionic Liquid for Flexible Zinc–Air Batteries**
Hongdae Lee, Yoonbin Kim, Won Il Kim, Gun Jang, Jung Woo Hong, Jun Su Kim, Chengang Pei, Jin Suk Byun, Sang Joon Lee, Sung Oh Moon, Young Soo Yun, Won-Chul Cho, **Byung-Hyun Kim**, and Ho Seok Park*
Chemical Engineering Journal 524, 169642 (2025) · IF 13.2, Top 3.0% (JCR 2024) · doi:10.1016/j.cej.2025.169642
- [54] **Bottom-Up Synthesis of 2D AlN Nanosheets with Superior Hydrolytic Resistance and Thermal Conductivity**
Wonyeong Lee†, Gyuchan Kim†, **Byung-Hyun Kim**, Haekyun Park, Sung-Joon Park, Chang-Min Yoon*, and Myeongjin Kim*
Small 21, e07445 (2025) · IF 12.1, Top 7.2% (JCR 2024) · doi:10.1002/smll.202507445
- [53] **Exploring Materials Data through Collaboration: 2024 KRICT ChemDX Hackathon**
Su-Hyun Yoo*, Andre K. Y. Low, Jose Recatala-Gomez, Harikrishna Sahu, Chiho Kim, Joonyoung F. Joung, Hoje Chun, Katerina A. Christofidou, Joshua Berry, Michail Minotakis, Kisung Kang, Kwangsoo Kim, Gaheun Shin, Hyunwoo Jang, Sanghyuk Lee, Minkyu Park, **Byung-Hyun Kim**, Kihyun Shin, Jungho Shin, Aloysius Soon, Joshua Schrier*, and Woosun Jang*
Journal of Materials Informatics 5, 54 (2025) · IF 5.6, Top 28.7% (JCR 2024) · doi:10.20517/jmi.2025.65
- [52] **Durable and Efficient Solar CO₂-to-CO Conversion Enabled by Single-Atom Ag on Zn₃(PO₄)₂ Cathode Coupled with a GaAs/Pt_{SA}@NiOOH Photoanode**
Maheswari Arunachalam, Kwangsoo Kim, Kug-Seung Lee, **Byung-Hyun Kim***, and Soon Hyung Kang*
Advanced Energy Materials 15, e02953 (2025) · IF 26.0, Top 2.5% (JCR 2024) · doi:10.1002/aenm.202502953
- [51] **Enhanced Oxygen Evolution Reaction on Upcycled LiCoO₂ via Structural Phase Transformation**
Greeshma Suresh†, Woowon Chung†, Min Soo Kim†, Gyuchan Kim†, M. Usman Ahmad, Jinha Shim, **Byung-Hyun Kim***, and Jin Ho Bang*
Advanced Sustainable Systems 9, e00733 (2025) · IF 6.1, Top 27.0% (JCR 2024) · doi:10.1002/adsu.202500733
- [50] **Heterointerface-Driven Electronic Modulation in MoO₂@N/Mo-ReS₂ Hybrid for Efficient Alkaline HER, OER, and Overall Water Splitting**
Manjinder Singh†, Jaejun Park†, Hayoung Kim†, Gyuchan Kim, Dunchan Cha, Dasu Ram Paudel, **Byung-Hyun Kim***, and Seunghyun Lee*
Small 21, 2505906 (2025) · IF 12.1, Top 7.2% (JCR 2024) · doi:10.1002/smll.202505906
- [49] **Rapid Flame Induced Dual-Metal Doping on WO₃ Electrode for Boosting Photo-Electrochemical Water Oxidation**
Seung Hun Roh†, Jaekyum Kim†, Won So, Yuankai Li, Won Tae Hong, Hyun Min Kwon, Sae Byeok Jo, Wooseok Yang, Byung-Keun Oh, Chan-Hwa Chung, Jongwook Park, Chisung Ahn*, **Byung-Hyun Kim***, and Jung Kyu Kim*
Energy Materials 5, 500128 (2025) · IF 11.2, Top 10.2% (JCR 2024) · doi:10.20517/energymater.2025.59

- [48] **Facet-Controlled Growth of Molybdenum Phosphide Single Crystals for Efficient Hydrogen Peroxide Synthesis**
Seo Hyun Kim†, Jeong-Hyun Kim†, Bogeun Park†, Hanhwi Jang, Jeong-Gyu Lee, Soonmin Yim, Jae Won Jeong, Seyoung Koo, Yeon Sik Jung, **Byung-Hyun Kim***, Min-Jae Choi*, and Hyeuk Jin Han*
Advanced Materials 37, 2500250 (2025) · [Inside Front Cover](#) · IF 26.8, Top 2.1% (JCR 2024) · [doi:10.1002/adma.202500250](#)
- [47] **Ligand Engineering of Co-N₄ Single-Atom Catalysts for Highly-Active and Stable Acidic Oxygen Evolution**
Taeyoung Jeong†, Kiwon Kim†, **Byung-Hyun Kim**, Sang-Il Choi, Chang Hyuck Choi*, Joonhee Kang*, and Myeongjin Kim*
Advanced Science 12, 2502230 (2025) · IF 14.1, Top 7.0% (JCR 2024) · [doi:10.1002/advs.202502230](#)
- [46] **Highly Selective Photoelectrochemical Glycerol Valorization toward Lactic Acid with Low-Valence Bimetallic Overlayer on CuWO₄**
Yuankai Li†, Jaekyum Kim†, Won Tae Hong, Jun Young Kim, Qian Lei, Hyungu Han, Unbeom Baeck, Dong Hyun Kim, Chang Hyuck Choi, **Byung-Hyun Kim***, Chan-Hwa Chung, and Jung Kyu Kim*
ACS Energy Letters 10, 2305 (2025) · [Cover](#) · IF 18.9, Top 4.1% (JCR 2024) · [doi:10.1021/acsenenergylett.5c00551](#)
- [45] **Interaction Study of Copper Ions and Polyvinyl Acetal (PVA) Brush during Copper Post-CMP Cleaning: Experimental and Density Functional Theory Study**
Sanjay Bisht, Maheepal Yadav, **Byung-Hyun Kim**, Tae-Gon Kim*, and Jin-Goo Park*
Applied Surface Science 695, 162858 (2025) · IF 6.9, Top 10.4% (JCR 2024) · [doi:10.1016/j.apsusc.2025.162858](#)
- [44] **Enhanced Electrochemical Performance of Aqueous Zn-Ion Batteries Based on Na₂V₆O₁₆·2H₂O Cathodes: Insights from DFT and Synchrotron X-ray Analysis**
Youngee So†, Huncheol Seo†, Seung Hwan Lee†, Eunseo Lee, Jinyoung Lee, Joonhee Kang, Young Yong Kim*, **Byung-Hyun Kim***, and Sungwook Mhin*
Journal of Materials Chemistry A 13, 8761 (2025) · IF 9.5, Top 13.6% (JCR 2024) · [doi:10.1039/D4TA08338E](#)
- [43] **Breakthrough Scalable Synthesis of Anti-coking Cs-Ni/CeO_x-Al₂O₃ Nanocatalysts for Optimal Dry Reforming Performance**
Kyung Hee Oh, Shin Wook Kang, Jin Gyu Lee, Jung-Il Yang, **Byung-Hyun Kim**, Chang Seop Hong*, and Ji Chan Park*
Nano Research 18, 94907116 (2025) · IF 9.0, Top 13.1% (JCR 2024) · [doi:10.26599/NR.2025.94907116](#)
- [42] **Optimizing KOH/cPVC Ratio for Improved CH₄ and CO₂ Adsorption Capacities of Porous Carbon Adsorbents**
Phuong Uyen Do, Kwangsoo Kim, **Byung-Hyun Kim**, and Chan Hyun Lee*
Chemistry of Materials 37, 1047 (2025) · IF 7.0, Top 22.0% (JCR 2024) · [doi:10.1021/acs.chemmater.4c02733](#)
- [41] **Synergistic Configuration of Binary Rhodium Single Atoms in Carbon Nanofibers for High-Performance Alkaline Water Electrolyzer**
Natarajan Logeshwaran†, Gyuchan Kim†, Pandiarajan Thangavel†, Sun Seo Jeon, Kaliannan Thiagarajan, Kampara Roopa Kishore, Hyunjo Lee, Inseok Seo, Hongseok Yun, Sungho Lee*, **Byung-Hyun Kim***, and Young Jun Lee*
Advanced Science 12, 2413176 (2025) · IF 14.1, Top 7.0% (JCR 2024) · [doi:10.1002/advs.202413176](#)
- [40] **Activating the Mn Single Atomic Center for an Efficient Actual Active Site of the Oxygen Reduction Reaction by Spin-State Regulation**
Kiwon Kim†, Gyuchan Kim†, Taeyoung Jeong, Wonyoung Lee, Yunho Yang, **Byung-Hyun Kim**, Bubryur Kim, Byeongyong Lee, Joonhee Kang*, and Myeongjin Kim*
Journal of the American Chemical Society 146, 34033 (2024) · IF 14.5, Top 7.6% (JCR 2023) · [doi:10.1021/jacs.4c13137](#)
- [39] **Time-Efficient Atmospheric Water Harvesting using Fluorophenyl Oligomer Incorporated MOFs**
Min Seok Kang†, Incheol Heo†, Sun Ho Park†, Jinhee Bae, Sangyeop Kim, Gyuchan Kim, **Byung-Hyun Kim**, Nak Cheon Jeong*, and Won Cheol Yoo*
Nature Communications 15, 9793 (2024) · IF 14.7, Top 5.6% (JCR 2023) · [doi:10.1038/s41467-024-53853-7](#)
- [38] **Sampling Rare Events using Nanostructures for Universal Pt Neural Network Potential**
Joonhee Kang*, **Byung-Hyun Kim**, Min Ho Seo, and Jehyun Lee
Current Applied Physics 66, 110 (2024) · IF 2.4, Top 53.4% (JCR 2023) · [doi:10.1016/j.cap.2024.07.005](#)
- [37] **Highly Reliable and Large-Scale Simulations of Promising Argyrodite Solid-State Electrolytes Using a Machine-Learned Moment Tensor Potential**
Ji Hoon Kim, Byeongsun Jun, Yong Jun Jang, Sun Ho Choi, Seong Hyeon Choi, Sung Man Cho, Yong-Gu Kim, **Byung-Hyun Kim**, and Sang Uck Lee*
Nano Energy 124, 109436 (2024) · IF 16.8, Top 5.3% (JCR 2023) · [doi:10.1016/j.nanoen.2024.109436](#)

- [36] **Coordination Engineering of N, O Co-Doped Cu Single Atom on Porous Carbon for High Performance Zinc Metal Anodes**
Kyungbin Lee†, Eun Ji Kim†, Jaekyum Kim, Keun Hee Kim, Young Jun Lee, Michael J. Lee, Kun Ryu, Sangyong Shin, Jaeyoung Choi, Seung Ho Kwon, Hyunjo Lee, Jung Kyu Kim, **Byung-Hyun Kim***, Bumjoon J. Kim*, and Seung Woo Lee*
Advanced Energy Materials 14, 2303803 (2024) · IF 24.4, Top 2.6% (JCR 2023) · doi:10.1002/aenm.202303803
- [35] **Novel Solid-State Synthesis of Surfactant- and Solvent-free Pd Tetrahedron Nanocatalysts**
Kyung Hee Oh, Kwangsoo Kim, Jin Gyu Lee, Nahyun Park, Hack-Keun Lee, Shin Wook Kang, Jung-Il Yang, Byeong-Seon An, Kang Hyun Park, Chang Seop Hong*, **Byung-Hyun Kim***, and Ji Chan Park*
Journal of Materials Chemistry A 12, 1233 (2024) · IF 10.8, Top 9.1% (JCR 2023) · doi:10.1039/d3ta06056j
- [34] **Highly Efficient Water-splitting Electrodes with Stable Operation at 3 A cm⁻² in Alkaline Media through Molecular Linker Assembly-induced All-in-one Structured NiMo and NiFe Electrocatalysts**
Youhyun Son, Jeongmin Mo, Euiju Yong, Jeongyeon Ahn, Gyuchan Kim, Wonyoung Lee, Cheong Hoon Kwon, Hyun Ju, Seung Woo Lee, **Byung-Hyun Kim***, Myeongjin Kim*, and Jinhan Cho*
Applied Catalysis B: Environmental 343, 123563 (2024) · IF 20.3, Top 0.6% (JCR 2023) · doi:10.1016/j.apcatb.2023.123563
- [33] **Unexpected Penetration of CO Molecule into Zeolitic Micropores Almost Plugged by CuCl via π -Complexation of CO-CuCl**
Chan Hyun Lee†*, Kwangsoo Kim†, Jisoo Kim, Kanghee Cho, Sang-Sup Han, Hyun Wook Kim, Ki Bong Lee, **Byung-Hyun Kim**, Jong Hyeok Park, Kyoungsoo Kim, and Jong-Ho Park*
ACS Applied Materials & Interfaces 15, 27411 (2023) · IF 9.5, Top 15.8% (JCR 2022) · doi:10.1021/acsami.3c04849
- [32] **An Electrochemically Active Textile Current Collector with a High Areal Capacity and a Strong Energy Recovery Effect Using an Interfacial Interaction Assembly**
Euiju Yong†, Donghyeon Nam†, Yangsoo Kim, Kwangsoo Kim, **Byung-Hyun Kim***, Yongmin Ko*, and Jinhan Cho*
Energy Storage Materials 60, 102813 (2023) · IF 20.4, Top 4.2% (JCR 2022) · doi:10.1016/j.ensm.2023.102813
- [31] **Structure-Controlled Carbon Hosts for Dendrite-Free Aqueous Zinc Batteries**
Kyungbin Lee†, Young Jun Lee†, Michael J. Lee, Junghun Han, Kun Ryu, Jeong An Kwon, Eun Ji Kim, Hyewon Kang, **Byung-Hyun Kim***, Bumjoon J. Kim*, and Seung Woo Lee*
Small 19, 2302334 (2023) · IF 13.3, Top 6.6% (JCR 2022) · doi:10.1002/smll.202302334
- [30] **Rational Design of a Stable Fe-rich Ni-Fe Layered Double Hydroxide for the Industrially Relevant Dynamic Operation of Alkaline Water Electrolyzers**
Muhammad Mehdi, Byeong-Seon An, Haesol Kim, Sechan Lee, Changsoo Lee, Myeongmin Seo, Min Wook Noh, Won-Chul Cho, Chang-Hee Kim, Chang Hyuck Choi, **Byung-Hyun Kim***, MinJoong Kim*, and Hyun-Seok Cho*
Advanced Energy Materials 13, 2204403 (2023) · Inside Front Cover · IF 27.8, Top 2.5% (JCR 2022) · doi:10.1002/aenm.202204403
- [29] **Electrochemical Partial Reduction of Ni(OH)₂ to Ni(OH)₂/Ni via Coupled Oxidation of an Interfacing NiAl Intermetallic Compound for Robust Hydrogen Evolution**
Young Hwa Yun†, Kwangsoo Kim†, Changsoo Lee†, Byeong-Seon An, Ji Hee Kwon, Sechan Lee, MinJoong Kim, Jongsu Seo, Jong Hyeok Park*, **Byung-Hyun Kim***, and Hyun-Seok Cho*
Journal of Energy Chemistry 82, 560 (2023) · IF 13.1, Top 2.1% (JCR 2022) · doi:10.1016/j.jechem.2023.03.023
- [28] **Colossal Dielectric Perovskites of Calcium Copper Titanate(CaCu₃Ti₄O₁₂) with Low-Iridium Dopants Enables Ultrahigh Mass Activity for the Acidic Oxygen Evolution Reaction**
Nguyen Thi Thu Thao†, Kwangsoo Kim†, Jeong Ho Ryu†, Byeong-Seon An, Arpan Kumar Nayak, Jin Uk Jang, Kyeong-Han Na, Won-Youl Choi, Ghulam Ali, Keun Hwa Chae, Muhammad Akbar, Kyung Yoon Chung, Hyun-Seok Cho, Jong Hyeok Park, **Byung-Hyun Kim***, and HyukSu Han*
Advanced Science 10, 2207695 (2023) · Inside Front Cover · IF 15.1, Top 6.8% (JCR 2022) · doi:10.1002/advs.202207695
- [27] **Crucial Role of Alkali Metal Ions and Si/Al ratio in Selective Adsorption of 1-Octene using Faujasite Zeolites**
Hui Seon Park†, Dong-Woo Cho†, Kwangsoo Kim, **Byung-Hyun Kim**, Jongkee Park, Chung-Yul Yoo*, and Taesung Jung*
Separation and Purification Technology 314, 123531 (2023) · IF 8.6, Top 8.1% (JCR 2022) · doi:10.1016/j.seppur.2023.123531
- [26] **A New Automated Synthesis of a Coke-resistant Cs-promoted Ni-supported Nanocatalyst for Sustainable Dry Reforming of Methane**
Kyung Hee Oh, Jin Hee Lee, Kwangsoo Kim, Hack-Keun Lee, Shin Wook Kang, Jung-Il Yang, Jong-Ho Park, Chang Seop Hong*-, **Byung-Hyun Kim***, and Ji Chan Park*
Journal of Materials Chemistry A 11, 1666 (2023) · Inside Front Cover · IF 11.9, Top 8.8% (JCR 2022) · doi:10.1039/D2TA08442B

- [25] **Structure-Controlled Graphene Electrocatalysts for High-Performance H₂O₂ Production**
 Kyungbin Lee†, Jeonghoon Lim†, Michael J. Lee, Kun Ryu, Hoyoung Lee, Jin Young Kim, Hyunchul Ju, Hyun-Seok Cho, **Byung-Hyun Kim**,
 Marta C. Hatzell*, Joonhee Kang*, and Seung Woo Lee*
Energy & Environmental Science 15, 2858 (2022) · [Inside Front Cover](#) · IF 39.7, Top 0.2% (JCR 2021) · [doi:10.1039/D2EE00548D](https://doi.org/10.1039/D2EE00548D)
- [24] **A 3D Hierarchical Host with Enhanced Sodiophilicity Enabling Anode-Free Sodium-Metal Batteries**
 Kyungbin Lee†, Young Jun Lee†, Michael J. Lee, Junghun Han, Jeonghoon Lim, Kun Ryu, Hana Yoon, **Byung-Hyun Kim***, Bumjoon J.
 Kim*, and Seung Woo Lee*
Advanced Materials 34, 2109767 (2022) · [Back Cover](#) · IF 32.1, Top 2.1% (JCR 2021) · [doi:10.1002/adma.202109767](https://doi.org/10.1002/adma.202109767)
- [23] **Role of Surface Steps in Activation of Surface Oxygen Sites on Ir Nanocrystals for Oxygen Evolution Reaction in Acidic Media**
 Myeongjin Kim†, Jinho Park†, Maoyu Wang, Qingxiao Wang, Moon J. Kim, Jin Young Kim, Hyun-Seok Cho, Chang-Hee Kim, Zhenxing Feng,
Byung-Hyun Kim*, and Seung Woo Lee*
Applied Catalysis B: Environmental 302, 120834 (2022) · IF 24.3, Top 0.9% (JCR 2021) · [doi:10.1016/j.apcatb.2021.120834](https://doi.org/10.1016/j.apcatb.2021.120834)
- [22] **First-Principles Based Machine-Learning Molecular Dynamics for Crystalline Polymers with van der Waals Interactions**
 Sung Jun Hong†, Hoje Chunt†, Jehyun Lee, **Byung-Hyun Kim**, Min Ho Seo, Joonhee Kang*, and Byungchan Han*
Journal of Physical Chemistry Letters 12, 6000 (2021) · IF 6.5, Top 6.8% (JCR 2020) · [doi:10.1021/acs.jpclett.1c01140](https://doi.org/10.1021/acs.jpclett.1c01140)
- [21] **Unravelling the K-Promotion Effect in Highly Active and Stable Fe₅C₂ Nanoparticles for Catalytic Linear α -Olefin Production**
 Jin Hee Lee†, Hack-Keun Lee†, Kwangsoo Kim, Geun Bae Rhim, Min Hye Youn, Heondo Jeong, Jong Hyeok Park, Dong Hyun Chun*,
Byung-Hyun Kim*, and Ji Chan Park*
Materials Advances 2, 1050 (2021) · [doi:10.1039/D0MA00920B](https://doi.org/10.1039/D0MA00920B)
- [20] **Understanding Synergistic Metal-Oxide Interactions of in situ Exsolved Metal Nanoparticles on a Pyrochlore Oxide Support for Enhanced Water Splitting**
 Myeongjin Kim*, Jinho Park, Hyun Ju, Jin Young Kim, Hyun-Seok Cho, Chang-Hee Kim, **Byung-Hyun Kim***, and Seung Woo Lee*
Energy & Environmental Science 14, 3053 (2021) · [Front Cover](#) · IF 38.5, Top 0.2% (JCR 2020) · [doi:10.1039/D0EE02935A](https://doi.org/10.1039/D0EE02935A)
- [19] **Sorption-Enhanced Thin Film Composites with Metal-Organic Polyhedral Nanocages for CO₂ Separation**
 Muhammad Sohail†, Heseong An†, Wanuk Choi, Jatinder Singh, Kanghoon Yim, **Byung-Hyun Kim**, Young Cheol Park, Jong Suk Lee*, and
 Hyunuk Kim*
Journal of Membrane Science 620, 118826 (2021) · IF 8.7, Top 3.9% (JCR 2020) · [doi:10.1016/j.memsci.2020.118826](https://doi.org/10.1016/j.memsci.2020.118826)
- [18] **Ion Irradiation Induced Surface Composition Modulation in Equiatomic Binary Alloys**
Byung-Hyun Kim*, Sang-Pil Kim, Joonhee Kang, Yong-Chae Chung, Kyung-Suk Kim, and Kwang-Ryeol Lee*
Applied Surface Science 540, 148103 (2021) · IF 6.7, Top 2.4% (JCR 2020) · [doi:10.1016/j.apsusc.2020.148103](https://doi.org/10.1016/j.apsusc.2020.148103)
- [17] **Facile Synthesis of a High Performance NiPd@CMK-3 Nanocatalyst for Mild Suzuki-Miyaura Coupling Reactions**
 Ji Chan Park†, Aram Kim†, Sanha Jang, Jung-Il Yang, Shin Wook Kang, Chan-Woo Lee, **Byung-Hyun Kim***, and Kang Hyun Park*
ChemCatChem 11, 991 (2019) · IF 4.5, Top 28.7% (JCR 2018) · [doi:10.1002/cctc.201801872](https://doi.org/10.1002/cctc.201801872)
- [16] **Multiscale Modeling of Agglomerated Ceria Nanoparticles: Interface Stability and Oxygen Vacancy Formation**
Byung-Hyun Kim, Jolla Kullgren*, Matthew J. Wolf, Kersti Hermansson*, and Peter Broqvist*
Frontiers in Chemistry 7, 203 (2019) · IF 3.8, Top 31.1% (JCR 2018) · [doi:10.3389/fchem.2019.00203](https://doi.org/10.3389/fchem.2019.00203)
- [15] **Indirect-to-Direct Band Gap Transition of Si Nanosheets: Effect of Biaxial Strain**
Byung-Hyun Kim†, Mina Park†, Gyubong Kim, Kersti Hermansson, Peter Broqvist, Heon-Jin Choi, and Kwang-Ryeol Lee*
Journal of Physical Chemistry C 122, 15297 (2018) · IF 4.5, Top 18.8% (JCR 2017) · [doi:10.1021/acs.jpcc.8b02239](https://doi.org/10.1021/acs.jpcc.8b02239)
- [14] **Functionalization Effect on a Pt/carbon Nanotube Composite Catalyst: A first-principles Study**
Byung-Hyun Kim, Kwang-Ryeol Lee, Yong-Chae Chung, and Mina Park*
Physical Chemistry Chemical Physics 18, 22687 (2016) · IF 4.4, Top 15.7% (JCR 2015) · [doi:10.1039/C5CP07737K](https://doi.org/10.1039/C5CP07737K)
- [13] **Reactive Molecular Dynamic Simulations of Early Stage of Wet Oxidation of Si (001) Surface**
 Mauludi Ariesto Pamungkas, **Byung-Hyun Kim**, and Kwang-Ryeol Lee*
Journal of Applied Physics 114, 073506 (2013) · IF 2.2, Top 24.6% (JCR 2012) · [doi:10.1063/1.4818941](https://doi.org/10.1063/1.4818941)

- [12] **A Molecular Dynamics Simulation Study on the Initial Stage of Si(001) Oxidation under Biaxial Strain**
Haining Cao, Mauludi Ariesto Pamungkas, **Byung-Hyun Kim**, and Kwang-Ryeol Lee*
Journal of Nanoscience and Nanotechnology 13, 1074 (2013) · doi:10.1166/jnn.2013.6120
- [11] **Effects of Suboxide Layers on the Electronic Properties of Si(100)/SiO₂ Interfaces: Atomistic Multi-scale Approach**
Byung-Hyun Kim, Gyubong Kim*, Kihoon Park, Mincheol Shin*, Yong-Chae Chung, and Kwang-Ryeol Lee
Journal of Applied Physics 113, 073705 (2013) · IF 2.2, Top 24.6% (JCR 2012) · doi:10.1063/1.4791706
- [10] **Effects of Interfacial Bonding in the Si-Carbon Nanotube Nanocomposite: A Molecular Dynamics Approach**
Byung-Hyun Kim*, Kwang-Ryeol Lee, Yong-Chae Chung, and June Gunn Lee
Journal of Applied Physics 112, 044312 (2012) · IF 2.2, Top 29.2% (JCR 2011) · doi:10.1063/1.4748133
- [9] **Interfacial Reaction-Dominated Full Oxidation of 5 nm Diameter Silicon Nanowires**
Ilsoo Kim, Tae-Eon Park, Ki-Young Lee, Ryong Ha, **Byung-Hyun Kim**, Yong-Chae Chung, Kwang-Ryeol Lee, and Heon-Jin Choi*
Journal of Applied Physics 112, 094308 (2012) · IF 2.2, Top 29.2% (JCR 2011) · doi:10.1063/1.4764004
- [8] **Atomic-Scale Simulations of Early Stage of Oxidation of Vicinal Si(001) Surfaces Using a Reactive Force-Field Potentials**
Kyung-Han Yun, Yubin Hwang, Heechae Choi, Eung-Kwan Lee, Geunsup Yoon, **Byung-Hyun Kim**, and Yong-Chae Chung*
Japanese Journal of Applied Physics 50, 10PF01 (2011) · IF 1.0, Top 64.0% (JCR 2010) · doi:10.1143/JJAP.50.10PF01
- [7] **Stress Evolution during the Oxidation of Silicon Nanowires in the Sub-10 nm Diameter Regime**
Byung-Hyun Kim, Mauludi Ariesto Pamungkas, Mina Park, Gyubong Kim, Kwang-Ryeol Lee*, and Yong-Chae Chung
Applied Physics Letters 99, 143115 (2011) · IF 3.8, Top 12.3% (JCR 2010) · doi:10.1063/1.3643038
- [6] **Reactive Molecular Dynamics Simulation of Early Stage of Dry Oxidation of Si(100) Surface**
Mauludi Ariesto Pamungkas, Minwoong Joe, **Byung-Hyun Kim**, and Kwang-Ryeol Lee*
Journal of Applied Physics 110, 053513 (2011) · IF 2.1, Top 28.4% (JCR 2010) · doi:10.1063/1.3632968
- [5] **Improved Binding between Copper and Carbon Nanotubes in a Composite using Oxygen-containing Functional Groups**
Mina Park, **Byung-Hyun Kim**, Sanghak Kim, Do-Suck Han, Gunn Kim, and Kwang-Ryeol Lee*
Carbon 49, 811 (2011) · IF 4.9, Top 8.2% (JCR 2010) · doi:10.1016/j.carbon.2010.10.019
- [4] **Anisotropic Rearrangement of the Substrate Atoms during Ar Bombardment on Pd(001) Surface**
Sang-Pil Kim, **Byung-Hyun Kim**, Haeri Kim, Kwang-Ryeol Lee*, Yong-Chae Chung, Jikeun Seo, and Jae-Sung Kim
Nuclear Instruments and Methods in Physics Research B 269, 2605 (2011) · IF 1.0, Top 35.7% (JCR 2010) · doi:10.1016/j.nimb.2011.07.093
- [3] **Atomic-Scale Investigation of the Ti/Al(001) Interface: A Molecular Dynamics Simulation**
Geunsup Yoon, Soon-Gun Lee, **Byung-Hyun Kim**, and Yong-Chae Chung*
Japanese Journal of Applied Physics 49, 06GJ14 (2010) · IF 1.1, Top 52.3% (JCR 2009) · doi:10.1143/JJAP.49.06GJ14
- [2] **Molecular Dynamics Simulation of the Thin Film Deposition of Co/Cu(111) with Pb Surfactant**
Byung-Hyun Kim and Yong-Chae Chung*
Journal of Applied Physics 106, 044304 (2009) · IF 2.2, Top 20.5% (JCR 2008) · doi:10.1063/1.3194309
- [1] **Atomic-Level Investigation for Surface Characteristics in a Co-Cu Multilayer System: Molecular Dynamics Simulation**
Byung-Hyun Kim and Yong-Chae Chung*
IEEE Transactions on Magnetics 44, 2903 (2008) · IF 1.0, Top 39.4% (JCR 2007) · doi:10.1109/TMAG.2008.2001520