

# Donghun Kim, Ph. D.

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Senior Researcher, Computational Science Research Center, KIST

## EDUCATION & CAREER

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### Computational Science Research Center, Korea Institute of Science and Technology (KIST)

2017.07–Present, Senior Researcher

2015.09–2017.06, Post-Doc (Alternative Military Service)–Supervisor: Dr. Sang Soo Han

### Massachusetts Institute of Technology (MIT)

2010.09–2015.08, Ph.D. Materials Science and Engineering (Minor in Teaching) –Supervisor: Prof. Jeffrey C. Grossman

### Pohang University of Science and Technology (POSTECH)

2006.03–2010.02, B.S. Materials Science and Engineering (GPA 4.13/4.3) –Highest GPA Graduate in School of Engineering

## EXPERTISE & RESEARCH INTEREST

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### Methodological Expertise

- Atomistic simulations (density functional theory, molecular dynamics, Monte Carlo)
- Artificial intelligence, machine learning, and data analytics

### Research Interest:

- Data/AI-enabled accelerations of material development (catalysis, photovoltaics, display)
- Machine learning interatomic potential
- Generative AI for material and synthesis predictions
- Intelligent material design laboratory (robotics/AI-based autonomous lab)

## JOURNAL PUBLICATION

\*Equal Contribution \*Corresponding

44 papers published (19 corresponding; 8 first-authored; 17 contributing)

3 manuscripts submitted for publications (3 corresponding; 0 contributing)

Google scholar citations = 2,897; h-index = 23

### Under Review

1. Unraveling Oxygen Vacancy-Driven Catalytic Selectivity and Hot Electron Generation on Heterointerfaces Using Nanostructured Platform  
GR Lee<sup>+</sup>, K Song<sup>+</sup>, D Hong<sup>+</sup>, J Ahn, Y Roh, M Kim, **D Kim**<sup>\*</sup>, YS Jung<sup>\*</sup>, JY Park<sup>\*</sup>  
Under Revision at **Nature Communications**
2. MaTableGPT: GPT-Based Table Data Extractor from Materials Science Literature  
GH Yi<sup>+</sup>, J Choi<sup>+</sup>, H Song<sup>+</sup>, O Miano, J Choi, K Bang, B Lee, SS Sohn, D Buttler, A Hiszpanski<sup>\*</sup>, SS Han<sup>\*</sup>, **D Kim**<sup>\*</sup>  
Under Review at **Advanced Science** (available at **arXiv:2406.05431**)
3. Simultaneous Enhancement of the Activity and Durability of the Oxygen Reduction Reaction Via Pd<sub>3</sub>Mo@Pt/C Catalysts  
J Yoo<sup>+</sup>, CH Chan<sup>+</sup>, SY Choi, D Hong, SY Park, K Bang, JM Kim, **D Kim**<sup>\*</sup>, SS Han<sup>\*</sup>, HM Lee<sup>\*</sup>  
Under Review at **Chem Catalysis**

### Published

1. OCTOPUS: Operation Control System for Task Optimization and Job Parallelization via a User-Optimal Scheduler

- HJ Yoo, KY Lee\*, **D Kim\***, SS Han\*  
**Nature Communications (Accepted)**
- Indirect-to-Direct Bandgap Transition in GaP Semiconductor through Quantum Shell Formation on ZnS Nanocrystals  
HJ Shin<sup>+</sup>, D Hong<sup>+</sup>, H Cho, H Jang, GY Kim, KM Song, MJ Choi\*, **D Kim\***, YS Jung\*  
**Nature Communications** 15:8125 (2024)
  - Enhancing Fuel Cell Durability with Heteroenergetic TaO<sub>x</sub>-Carbon Support  
S Choi<sup>+</sup>, D Hong<sup>+</sup>, JH Noh, J Yoo, C Lee, K Bang, JM Kim, EA Cho, SS Han\*, **D Kim\***, HM Lee\*  
**ACS Energy Letters** 9, 4265 (2024)
  - Bespoke Metal Nanoparticle Synthesis at Room Temperature and Discovery of Chemical Knowledge on Nanoparticle Growth via Autonomous Experimentations  
HJ Yoo<sup>+</sup>, N Kim<sup>+</sup>, HS Lee, DH Kim, L Tiong, CS Kim, SY Lee, KY Lee\*, **D Kim\***, SS Han\*  
**Advanced Functional Materials** 34, 23125612 (2024) – Selected as Front Cover
  - Machine Vision-based Detections of Transparent Chemical Vessels Toward the Safe Automations of Material Synthesis  
L Tiong<sup>+</sup>, HJ Yoo<sup>+</sup>, NY Kim, CS Kim, KY Lee\*, SS Han\*, **D Kim\***  
**npj Computational Materials** 10, 42 (2024)
  - Inverse Design for Materials Discovery from Multidimensional Electronic Density of States  
K Bang<sup>+</sup>, J Kim<sup>+</sup>, D Hong<sup>+</sup>, **D Kim\***, SS Han\*  
**Journal of Materials Chemistry A** 12, 6004 (2024)
  - Efficient and Sustainable Water Electrolysis Achieved by Excess Electron Reservoir Enabling Charge Replenishment to Catalysts  
GR Lee<sup>+</sup>, J Kim<sup>+</sup>, D Hong<sup>+</sup>, YJ Kim, HJ Han, H Jang, CG Hwang, **D Kim\***, JY Kim\*, Y Jung\*  
**Nature Communications** 14:5402 (2023)
  - Machine Learning-Enabled Explorations of the Electrochemical Stability of Real-Scale Metallic Nanoparticles  
K Bang, D Hong, Y Park, **D Kim\***, SS Han\*, HM Lee\*  
**Nature Communications** 14:3004 (2023)
  - Deep Learning of Electrochemical CO<sub>2</sub> Conversion Literature Reveals Research Trends and Directions  
J Choi<sup>+</sup>, K Bang<sup>+</sup>, S Jang, JW Choi, J Ordonez, D Buttler, A Hiszpanski, TYJ Han, SS Sohn, B Lee, KR Lee, SS Han\*, **D Kim\***  
**Journal of Materials Chemistry A** 11, 17628 (2023)
  - Predicting Failure Progressions of Structural Material via Deep Learning Based on Void Topology  
L Tiong<sup>+</sup>, G Lee<sup>+</sup>, GH Yi, SS Sohn\*, **D Kim\***  
**Acta Materialia** 250, 118862 (2023)
  - Machine Learning Filters Out Efficient Electrocatalysts in the Massive Ternary Alloy Space for Fuel Cells  
Y Park<sup>+</sup>, CG Hwang<sup>+</sup>, K Bang, D Hong, H Nam, SH Kwon, BC Yeo, D Go, J An, BK Ju, SH Kim, JY Byun, SY Lee, SY Lee, JM Kim\*, **D Kim\***, SS Han\*, HM Lee\*  
**Applied Catalysis B: Environmental** 339, 123128 (2023)
  - Atomistic Origin of Mechanochemical NH<sub>3</sub> Synthesis on Fe Catalysts  
HW Lee<sup>+</sup>, GU Jeong<sup>+</sup>, MC Kim, **D Kim\***, S Kim\*, SS Han\*  
**International Journal of Hydrogen Energy** 48, 3931 (2023)
  - Solid-Solution Alloying of Immiscible Pt and Au Boosts Catalytic Performance for H<sub>2</sub>O<sub>2</sub> Direct Synthesis  
HW Lee<sup>+</sup>, H Nam<sup>+</sup>, GH Han<sup>+</sup>, YH Cho, BC Yeo, MC Kim, **D Kim\***, KY Lee\*, SY Lee\*, SS Han\*

- Acta Materialia** 205, 116563 (2021)
14. Deep Learning-Based Prediction of Material Properties Using Chemical Compositions and Diffraction Patterns as Experimentally Accessible Inputs  
J Kim<sup>†</sup>, L Tiong<sup>†</sup>, **D Kim**<sup>\*</sup>, SS Han<sup>\*</sup>  
**Journal of Physical Chemistry Letters** 12, 8376 (2021)
  15. High-Throughput Computational-Experimental Screening Protocol for the Discovery of Bimetallic Catalysts  
BC Yeo<sup>†</sup>, H Nam<sup>†</sup>, H Nam, MC Kim, HW Lee, **D Kim**, KY Lee, SY Lee<sup>\*</sup>, SS Han<sup>\*</sup>  
**npj Computational Materials** 7, 137 (2021)
  16. Three-in-One Strategy to Improve both Catalytic Activity and Selectivity: Nonconcentric Pd-Au Nanoparticles  
HW Lee, E Jung, GH Han, MC Kim, **D Kim**, KY Lee<sup>\*</sup>, SS Han<sup>\*</sup>, T. Yu<sup>\*</sup>  
**Journal of Physical Chemistry Letters** 12, 11098 (2021)
  17. Accelerated Mapping of Electronic Density of State Patterns of Metallic Nanoparticles Via Machine-Learning  
K Bang, BC Yeo, **D Kim**, SS Han<sup>\*</sup>, HM Lee<sup>\*</sup>  
**Scientific Reports** 11, 11604 (2021)
  18. Identification of Crystal Symmetry from Noisy Diffraction Patterns by A Shape Analysis and Deep Learning  
L Tiong<sup>†</sup>, J Kim<sup>†</sup>, SS Han<sup>\*</sup>, **D Kim**<sup>\*</sup>  
**npj Computational Materials** 6, 196 (2020)
  19. Artificial Intelligence to Accelerate the Discovery of N<sub>2</sub> Electroreduction Catalysts  
M Kim<sup>†</sup>, BC Yeo<sup>†</sup>, Y Park, HM Lee, SS Han<sup>\*</sup>, **D Kim**<sup>\*</sup>  
**Chemistry of Materials** 32, 709 (2020)
  20. Hydrogen-Bonding-Mediated Enhancements of Bio-inspired Electrochemical Nitrogen Reduction on Cu<sub>2-x</sub>S Catalysts  
MC Kim, HJ Nam, JH Choi, HS Kim, HW Lee, **D Kim**, J Kong, SS Han<sup>\*</sup>, SY Lee<sup>\*</sup>, HS Park<sup>\*</sup>  
**ACS Catalysis** 10, 10577 (2020)
  21. Self-Assembled Heterojunction of Metal Sulfides for Improved Photocatalysis  
S Khan, H Choi, **D Kim**, SY Lee, Q Zhu, J Zhang, S Kim<sup>\*</sup>, SH Cho<sup>\*</sup>  
**Chemical Engineering Journal** 395, 125092 (2020)
  22. Mapping Point Defects of Brookite TiO<sub>2</sub> for Photocatalytic Activity Beyond Anatase Phase and P25  
H Choi<sup>\*</sup>, S Khan, M Je, **D Kim**, S Lee, S.-H. Cho<sup>\*</sup>, T. Song<sup>\*</sup>  
**Journal of Physical Chemistry C** 124, 10376 (2020)
  23. Suppressing Interfacial Dipoles to Minimize Open-Circuit Voltage Loss in Quantum Dot Photovoltaics  
H Lim<sup>†</sup>, **D Kim**<sup>†</sup>, MJ Choi, EH Sargent, YS Jung<sup>\*</sup>, JY Kim<sup>\*</sup>  
**Advanced Energy Materials** 9, 1901938 (2019) – Selected as Front Cover
  24. Unlocking the Potential of Nanoparticles Composed of Immiscible Elements for Direct H<sub>2</sub>O<sub>2</sub> Synthesis  
**D Kim**<sup>†</sup>, H Nam<sup>†</sup>, YH Cho<sup>†</sup>, BC Yeo<sup>†</sup>, SH Cho, JP Ahn, KY Lee<sup>\*</sup>, SY Lee<sup>\*</sup>, SS Han<sup>\*</sup>  
**ACS Catalysis** 9, 8702 (2019)
  25. Medium-Range Order in Amorphous Ices Revealed by Persistent Homology  
S Hong, **D Kim**<sup>\*</sup>  
**Journal of Physics: Condensed Matter** 31, 455403 (2019)

26. Electronic Structural Origin of the Catalytic Activity Trend of Transition Metals for Electrochemical Nitrogen Reduction  
BC Yeo, J Kong, **D Kim**, WA Goddard III, HS Park\*, SS Han\*  
**Journal of Physical Chemistry C** 123, 31026 (2019)
27. Pattern Learning Electronic Density of States  
BC Yeo, **D Kim**, C Kim, SS Han\*  
**Scientific Reports** 9, 5879 (2019)
28. Electron-Hole Separation in Ferroelectric Oxides for Efficient Photovoltaic Responses  
D Kim, H Han, JH Lee, JW Choi, JC Grossman, HM Jang\*, **D Kim\***  
**Proceedings of the National Academy of Sciences (PNAS)** 115, 6566 (2018)
29. Origins of the Stokes Shift in PbS Quantum Dots: Impact of Polydispersity, Ligands, and Defects  
Y Liu\*, **D Kim\***, OP Morris, D Zhitomirsky, JC Grossman\*  
**ACS Nano** 12, 2838 (2018)
30. Engineering the Work Function of Solution-Processed Electrodes of Silver Nanocrystal Thin Film through Surface Chemistry Modification  
M Seong, H Kim, SW Lee, **D Kim\***, SJ Oh\*  
**APL Materials** 6, 121105 (2018)
31. Atomistic Sodiation Mechanism of Phosphorene-Graphene Heterostructure for Sodium-Ion Batteries Determined by First-Principles Calculations  
HW Lee, H Jung, BC Yeo, **D Kim**, SS Han\*  
**Journal of Physical Chemistry C** 122, 20653 (2018)
32. Dissimilar Anisotropy of Electron Versus Hole Bulk Transport in Anatase TiO<sub>2</sub>: Implications for Photocatalysis  
**D Kim**, BC Yeo, D Shin, H Choi, S Kim, N Park, SS Han\*  
**Physical Review B** 95, 045209 (2017)
33.  $\beta$ -CuGaO<sub>2</sub> as a Strong Candidate Material for Efficient Ferroelectric Photovoltaics  
S Song\*, **D Kim\***, HM Jang\*, BC Yeo, SS Han, CS Kim, JF Scott  
**Chemistry of Materials** 29, 7596 (2017)
34. Defect Engineering Toward Strong Photocatalysis of Nb-Doped Anatase TiO<sub>2</sub>: Computational Predictions and Experimental Verifications  
S Khan, H Cho, **D Kim**, SS Han, KH Lee, SH Cho\*, T Song\*, H Choi\*  
**Applied Catalysis B: Environmental** 206, 520 (2017)
35. Impact of Mg-Doping Site Control in the Performance of Li<sub>4</sub>Ti<sub>5</sub>O<sub>12</sub> Li-Ion Battery Anode: First-Principles Predictions and Experimental Verifications  
H Cho, H Son, **D Kim**, M Lee, S Boateng, H Choi\*, T Song\*, KH Lee\*  
**Journal of Physical Chemistry C** 121, 14994 (2017)
36. Photovoltaic Performance of PbS Quantum Dots Treated with Metal Salts  
DK Ko, A Maurano, SK Suh, **D Kim**, GW Hwang, JC Grossman, V Bulović\*, MG Bawendi\*  
**ACS Nano** 10, 3382 (2016)
37. High-Throughput Screening to Investigate the Relationship between the Selectivity and Working Capacity of Porous Materials for Propylene/Propane Adsorptive Separation  
BC Yeo, **D Kim**, H Kim, SS Han\*  
**Journal of Physical Chemistry C** 120, 24224 (2016)
38. Identifying and Eliminating Emissive Sub-Bandgap States in Thin Films of PbS Nanocrystals  
GW Hwang, **D Kim**, JM Cordero, MWB Wilson, CHM Chuang, JC Grossman, MG Bawendi\*

- Advanced Materials** 27, 4481 (2015)
39. Energy Level Modification in Lead Sulfide Quantum Dot Thin Films through Ligand Exchange  
PR Brown\*, D Kim\*, RR Lunt, N Zhao, MG Bawendi, JC Grossman\*, V Bulović\*  
**ACS Nano** 8, 5863 (2014)
  40. Role of Ultrathin Metal Fluoride Layer in Organic Photovoltaic Cells: Mechanism of Efficiency and Lifetime Enhancement  
KG Lim, MR Choi, JH Kim, D Kim, GH Jung, Y Park\*, JL Lee, TW Lee\*  
**ChemSusChem** 7, 1125 (2014)
  41. Impact of Stoichiometry on the Electronic Structure of PbS Quantum Dots  
D Kim, DH Kim, JH Lee, JC Grossman\*  
**Physical Review Letters (PRL)** 110, 196802 (2013)
  42. Controlling Surface Enrichment in Polymeric Hole Extraction Layers to Achieve High-Efficiency Organic Photovoltaic Cells  
D Kim, KG Lim, JH Park, TW Lee\*  
**ChemSusChem** 5, 2053 (2012)
  43. Approaches Toward Efficient and Stable Electron Extraction Contact in Organic Photovoltaic Cells: Inspiration from the Organic Light-Emitting Diodes  
TW Lee\*, KG Lim, D Kim  
**Electronic Materials Letters** 6, 4150 (2010)
  44. Curvilinear Electronics Formed Using Silicon Nanomembrane Circuits and Elastomeric Transfer Elements  
HC Ko, G Shin, S Wang, M Stoykovich, JW Lee, D Kim, JS Ha\*, Y Huang\*, K Hwang, JA Rogers\*  
**Small** 5, 2703 (2009)

## **PATENT**

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### **US Patent (등록 4 건, 출원 3 건)**

1. System and Method for Operating Laboratory Based on Modular Experiment Process. SS Han, D Kim, HJ Yoo, US Application No. 18,741,132
2. Modular Experiment Automation System and Method of Operating the Same. SS Han, D Kim, HJ Yoo, NY Kim, SY Lee, US Application No. 18,475,100
3. Method and Apparatus for Diagnosing Error of Object Placement Using Artificial Neural Network. D Kim, SS Han, L Tjong, HJ Yoo, US Application No. 18,334,030
4. Method and Electronic Apparatus for Predicting Electronic Structure of Material, SS Han, BC Yeo, D Kim, S Kim, US Patent Registration No. 11,475,340
5. Immiscible Composite Catalyst for Synthesis of Hydrogen Peroxide and Methods for Synthesizing of Hydrogen Peroxide Using the Same. SS Han, D Kim, SY Lee, H Nam. US Patent Registration No. 10,888,843
6. Method and Electronic Apparatus for Predicting Electronic Structure of Material. SS Han, BC Yeo, C Kim, D Kim. US Patent Registration No. 11,113,611
7. Eliminating Emissive Sub-Bandgap States in Nanocrystals. GW Hwang, D Kim, JM Cordero, MWB Wilson, CHM Chuang, JC Grossman, MG Bawendi. US Patent Registration No. 10,109,760

### **Korea Patent (등록 8 건, 출원 4 건)**

1. 불소가 도핑된 주석산화물 담지체를 이용한 수전해용 촉매 및 그 제조방법. 김종민, 백새얀, 김민석, 이성수, 김동훈, 한상수, 홍두선, 이승용, 조소혜, 장호성, 최재원, 황창규, 문준희, 전철호. 출원번호 10-2024-0079668

2. 실험공정 모듈화 기반의 실험실 운영 시스템 및 방법. 한상수, **김동훈**, 유혁준. 출원번호 10-2024-0038420
3. 모듈형 실험 자동화 시스템 및 이의 동작하는 방법. 한상수, **김동훈**, 유혁준, 김나연, 이승용. 출원번호 10-2023-0081255
4. 인공신경망을 이용하여 객체 배치 오류를 진단하는 방법 및 장치. **김동훈**, 한상수, 레슬리 칭오, 유혁준, 김나연. 출원번호 10-2023-0059043
5. 금속재료의 기계적 물성을 예측하는 방법 및 전자 장치. **김동훈**, 손석수, Leslie Tiong, 이건직. 등록번호 10-2515351
6. 촉매의 활성도를 예측하는 방법 및 전자장치. **김동훈**, 한상수, 김명준, 여병철. 등록번호 10-2402507
7. 화학적 촉매를 전산 모사하는 장치 및 전산 모사하는 방법. 김승철, 한상수, 이광렬, **김동훈**. 등록번호 10-2293346
8. 소재의 전자구조를 예측하는 방법 및 전자장치. 한상수, 여병철, **김동훈**, 김승철. 등록번호 10-2103548; 10-2103551
9. 과산화수소 합성용 촉매 및 이를 이용한 과산화수소 합성 방법. 한상수, **김동훈**, 이승용, 남효빈. 등록번호 10-2002482
10. 합금 촉매 후보 선정 방법. 한상수, 여병철, **김동훈**. 등록번호 10-2041226
11. 과산화수소 합성용 촉매 및 이를 이용한 과산화수소 합성 방법. 이승용, 한상수, 남효빈, **김동훈**, 조소혜, 장호성. 등록번호 10-2044382
12. 소재 전자구조 예측 머신러닝 방법 및 이를 지원하는 전자 장치. 한상수, 여병철, 김찬수, **김동훈**. 등록번호 10-1943518

## INVITED TALK

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1. 대한금속재료학회 특별심포지움 (소재연구데이터 심포지움) 초청강연 (2024.10)
2. Wiley Forum 초청강연 (2024.10)
3. 한국에너지기술연구원(KIER) 초청강연 (2024.10)
4. 대한금속재료학회 소재기술 지능화 · 자동화 워크숍 초청강연 (2024.09)
5. 대한금속재료학회 인공지능재료과학분과 하계단기강좌 초청강의 (2024.07)
6. 대한금속재료학회 전산재료과학분과 여름학교 초청강의 (2024.06)
7. 포스코홀딩스 미래기술연구원 초청강연 (2023.11)
8. 카이스트 신소재공학과 초청강의 (2023.11)
9. 한화솔루션 초청강연 (2023.11)
10. 부경대학교 에너지자원공학과 초청강연 (2023.11)
11. 대한금속재료학회 추계학술대회 초청발표 (2023.10)
12. 한국표준과학연구원(KRISS) 초청강연 (2023.09)
13. 대한금속재료학회 인공지능재료과학분과 하계단기강좌 강연 (2023.08)
14. 국민대학교 신소재공학과 초청강연 (2022.12)
15. 포스텍 신소재공학과 초청강연 (2022.12)
16. ENGE2022 학회 튜토리얼 강의 (재료과학 문제 해결을 위한 머신러닝 방법론) (2022.11)
17. 버츰어랩 katalitic 워크숍 초청발표 (2022.11)
18. 대한금속재료학회 추계학술대회 디지털혁신심포지움 초청발표 (2022.10)
19. 서울대학교 신소재공학과 초청강연 (2022.08)
20. 한양대학교 원자력공학과 초청강연 (2022.06)
21. 한국부식방식학회 초청강연 (2022.01)
22. 국민대 신소재공학과 초청강연 (2021.11)
23. 대한금속재료학회 추계학술대회 초청강연 (2021.10)
24. 한밭대 신소재공학과 초청강연 (2021.09)
25. UNIST 에너지공학과 초청강연 (2021.05)
26. 카이스트 신소재공학과 초청강의 (2020.12)

27. 한국세라믹학회 추계학술대회 초청강연 (2020.11)
28. 고려대학교 신소재공학부 초청강연 (2020.11)
29. 대한금속재료학회 추계학술대회 초청강연 (2020.10)
30. 한국생산기술연구원 초청강연 (2020.09)
31. 나노코리아 퍼블릭세션 초청강연 (2020.07)
32. 대한금속재료학회 인공지능재료과학분과 하계단기강좌 초청강연 (2020.07)
33. UNIST 에너지공학과 초청강연 (2020.05)
34. International Conference of Molecular Simulation (ICMS2019) 초청강연 (2019.11)
35. 나노코리아 2019 초청강연 (2019.07)
36. 국민대 신소재공학과 초청강연 (2019.06)
37. 광주과학기술원 신소재공학과 초청강연 (2019.05)
38. 카이스트 신소재공학과 초청강연 (2019.05)
39. 대한금속재료학회 춘계학술대회 전산재료과학분과 초청강연 (2019.04)
40. 서울대학교 재료공학부 초청강연 (2019.04)
41. 카이스트 신소재공학과 초청강연 (2018.12)
42. 서울대학교 재료공학부 초청강연 (2018.12)
43. ENGE 2018 초청강연 (2018.11)
44. 한국고등과학원(KIAS) 초청강연 (2018.10)
45. The 21<sup>st</sup> Asian Workshop on First-Principles Electronic Structure Calculations 초청강연 (2018.10)
46. The 12<sup>th</sup> KIAS Conference of Electronic Structure Calculation 초청강연 (2018.06)
47. 카이스트 신소재공학과 초청강연 (2018.05)
48. UNIST 물리학과 초청강연 (2018.05)
49. 포스텍 신소재공학과 초청강연 (2016.09)
50. 카이스트 EEWS 초청강연 (2016.06)
51. KIST 계산과학연구소 초청강연 (2014.06)

## PROJECT FUNDING

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1. (참여) 장수명 연료전지용 고효율 가역적 재생가능형 라디칼 스캐빈저 제조 기술 개발, 한국연구재단 (24.07-25.12, 7.5 억)
2. (참여) 그린수소 생산용 슈퍼축매 데이터 HUB, 한국연구재단 (24.07-25.12, 22.5 억)
3. (참여) 고이온전도성 고체 전해질 설계용 uncertainty 평가 기반의 초정밀 범용 AI 기술 개발, 한국연구재단 (24.04-25.12, 9.2 억)
4. (참여) 기후환경 소재 설계용 AI 분석 추론 기술 개발, KIST (24.01-26.12, 16 억)
5. (참여) 수전해 촉매 및 디스플레이용 나노입자 합성을 위한 AI 스마트 연구실 개발, 한국연구재단 (22.04-27.12, 54 억)
6. (참여) AI 기반 에너지 환경 소재 데이터 수집 및 활용기술 개발, 한국연구재단 (21.06-27.12, 20.2 억)
7. (책임) 인공지능 자연어처리 기법을 이용한 촉매문헌 데이터 추출 및 지식베이스 구축, KIST (21.04-24.12, 5.4 억)
8. (참여) 재료의 표면과 계면에 대한 전산모사와 기계학습 활용 플랫폼 개발, KIST (21.01-23.12, 36 억)
9. (참여) 에너지 및 환경 소재 데이터 수집관리, 한국연구재단 (20.09-21.03, 1.2 억)
10. (책임) 데이터 모양 분석을 통한, 재료 파괴시점 예측, 삼성미래기술육성사업 (19.12-23.05, 9 억)
11. (참여) 융합형 소재 빅데이터 플랫폼 개발 및 생태계 구축, 한국연구재단 (18.08-20.12, 13.5 억)
12. (참여) 소재-전자구조 양방향 맵핑 플랫폼 개발, 삼성미래기술육성사업 (18.06-23.05, 15 억)
13. (참여) 테마형 웹플랫폼 개발용 나노구조 모델링 및 전산모사 기법 집적화 기술 개발, 한국연구재단 (18.03-21.05, 13.3 억)

14. (참여) 이산화탄소 환원 촉매 설계용 머신러닝 플랫폼 개발, LG 전자 소재기술원 (17.12-19.05, 2 억)
15. (참여) 데이터 기반 R&D 환경 구축 사업, KIST (17.08-18.12, 10 억)
16. (책임) 양자점 물질의 전기적 및 광학적 성질 이해를 통한 태양전지 성능 개선, KIST (17.07-18.07, 0.2 억)
17. (참여) 데이터 기반 광촉매 소재 설계 기술 개발, KIST (17.01-19.12, 34 억)
18. (참여) 계산과학-조합실험-첨단분석기술 기반 양자 알케미 촉매 개발, 한국연구재단 (16.05-21.12, 90 억)
19. (참여) 계층 구조 광촉매 설계를 위한 멀티스케일 시뮬레이션 기술 개발, KIST (15.01-16.12, 29.5 억)

## **TECH. TRANSFER (기술이전)**

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Technology transfer to Virtual Lab Inc. (주식회사 버추얼랩) of machine learning softwares

Transfer object: An ML software to predict catalytic properties of real-scale nanoparticles

Period: 2021.06-2021.09

## **AWARD & SCHOLARSHIP**

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KIST Excellent Research Team of the Year (우수연구개발팀 상), KIST, 2024

KIST Researcher of the Month (이달의 KIST 인 상), KIST, 2023

KIST Young Fellow, KIST, 2020

Award from Chairman of the Board (이사장상), NST (국가과학기술연구회), 2020

John Wulff Award for Excellence in Teaching (Best TA of the Year), MIT, 2014

Global Top Talent Award, Hyundai Motors, 2014

Samsung Scholarship (\$250K of 5 years for Ph. D. Program), Samsung Foundation, 2010-2015

The Highest GPA Graduate in School of Engineering, POSTECH, 2010

Presidential Science Scholarship (\$40K of 4 years), Korea Government, 2006-2010

Merit-Based Scholarship to Top Student of Department (5 times), POSTECH, 2006-2010

## **PROFESSIONAL ACTIVITY & SERVICE**

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**Conference Organizing Committee:** International Conference on Molecular Simulations (ICMS2019), NanoKorea2022, ENGE2022, NanoKorea2024, ENGE2024

**Conference Symposium Activity:** AI Symposium of the Korean Institute of Metals and Materials (대한금속재료학회 인공지능재료과학분과, 총무 2020-2024, 부위원장 2024-Present)

## **REFERENCE**

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