

# *Curriculum Vitae*

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## **Professional experience**

- **02/27/2023-present**  
Assistant Professor, Department of Energy Science, Sungkyunkwan University, Korea
- **01/09/2021-02/26/2023**  
Assistant Professor, Department of Chemistry, Chungnam National University, Korea
- **01/12/2020-30/08/2021**  
Postdoctoral Fellow of National Research Foundation of Korea,  
Yusuf Hamied Department of Chemistry, University of Cambridge, United Kingdom  
Research Group: Prof. Angelos Michaelides
- **16/12/2019-30/11/2020**  
Postdoctoral Researcher, ETH Zürich/USI, Switzerland  
Research Group: Prof. Michele Parrinello
- **13/02/2019-12/12/2019**  
Postdoctoral Researcher, Ulsan National Institute of Science and Technology (UNIST), Korea  
Research Group: Prof. Kwang S. Kim
- **01/12/2016-28/02/2017**  
Visiting scholar, Rutgers University, U.S.A.  
Development of non-equilibrium Anderson impurity solver on the Keldysh contour.  
Research Group: Prof. Kristjan Haule

## **Education**

- **01/09/2014-12/02/2019**  
Ph.D., Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST)  
Supervisor: Prof. Kwang S. Kim  
Dissertation title: "*First-Principles calculation of energy materials*"
- **01/09/2012-08/08/2014**  
M.S. Department of Electrical & Electronic Engineering, Pohang University of Science and Technology (POSTECH)  
Supervisor: Prof. Jae Koo Lee  
Dissertation title: "*Linear and Nonlinear Landau Damping using Particle-in-Cell Simulation*"
- **01/03/2007-10/08/2012**  
B.S. Department of Electrical & Electronic Engineering, Pohang University of Science and Technology (POSTECH)

## **Publications**

1. **C. W. Myung\***, A. Hajibabaei, J. Cha, M. Ha, & K. S. Kim, Challenges, Opportunities, and Prospects in Metal Halide Perovskites from Theoretical and Machine Learning Perspectives. *Adv. Energy Mater.* **12**, 2202279 (2022). DOI: 10.1002/aenm.202202279

2. M. Ha, A. Hajibabaei, D. Y. Kim, A. N. Singh, J. Yun, **C. W. Myung\***, & K. S. Kim\*(co-corresponding author), Al-doping driven suppression of capacity and voltage fadings in 4d-element containing Li-ion-battery cathode materials: machine learning and density functional theory. *Adv. Energy Mater.* **12**, 2201497 (2022).
3. N. Clark, D. J. Kelly, M. Zhou, Y. Zhou, **C. W. Myung**, D. G. Hopkinson, C. Schran, A. Michaelides, R. Gorbachev, S. J. Haigh, Tracking single adatoms in liquid in a transmission electron microscope. *Nature* **609**, 942–947 (2022).
4. **C. W. Myung**, B. Hirshberg & M. Parrinello, Prediction of a supersolid phase in high-pressure deuterium. *Phys. Rev. Lett.* **128**, 045301 (2022).
5. M. Ha, D. Y. Kim, M. Umer, V. Gladkikh, **C. W. Myung\***, Kwang S. Kim\*(co-corresponding author), Tuning metal single atoms embedded in  $N_xC_y$  moieties toward high-performance electrocatalysis. *Energy Environ. Sci.* **14**, 3455 (2021).
6. **C. W. Myung\*** & K. S. Kim\*, Anharmonicity-Driven Rashba Cohelical Excitons Break Quantum Efficiency Limitation. *Adv. Mater.* **33**, 2005400 (2021).
7. J. Kim, Kwang S. Kim\*, & **C. W. Myung\***(co-corresponding author) Efficient electron extraction of SnO<sub>2</sub> electron transport layer for lead halide perovskite solar cell. *npj Computational Mater.* **6**, 100 (2020).
8. M. Harzandi, S. Shadman, M. Ha, **C. W. Myung\***, D. Y. Kim, H. J. Park, S. Sultan, W. Lee, P. Thangavel, W. J. Byun, S.-H. Lee, J. N. Tiwari\*, T. J. Shin, Z. Lee, J. S. Lee, K. S. Kim\*(co-corresponding author), Immiscible bi-metal single-atoms driven synthesis of electrocatalysts having superb mass-activity and durability. *Applied Catalysis B: Environmental* **270**, 118896 (2020).
9. Y. Park<sup>†</sup>, A. Jana<sup>†</sup>, **C. W. Myung**<sup>†</sup>, T. S. Yoon, T. J. Puchtler, C. C. Kocher, R. A. Taylor & K. S. Kim (<sup>†</sup>equally contributed). Enhanced photoluminescence quantum yield of MAPbBr<sub>3</sub> nanocrystals by passivation using graphene. *Nano Research* **13**, 932–938 (2020).
10. S. Sultan, M. Ha, D. Y. Kim, J. N. Tiwari\*, **C. W. Myung\***, A. Meena, T. J. Shin, K. H. Chae, & K. S. Kim\* (\*co-corresponding), Superb water splitting activity of the electrocatalyst Fe<sub>3</sub>Co(PO<sub>4</sub>)<sub>4</sub> designed with computation-aid. *Nat. Commun.* **10**, 5195 (2019).
11. **C. W. Myung**, G. Lee & K. S. Kim, La-doped BaSnO<sub>3</sub> electron transport layer for perovskite solar cells, *J. Mater. Chem. A* **6**, 23071-23077 (2018).
12. **C. W. Myung**, S. Javaid, K. S. Kim & G. Lee, Rashba-Dresselhaus effect in inorganic/organic lead iodide perovskite interfaces. *ACS Energy Lett.* **3**, 1294-1300 (2018).
13. **C. W. Myung**, J. Yun, G. Lee & K. S. Kim, A new perspective on the role of A-site cations in perovskite solar cells. *Adv. Energy Mater.* **8**, 1702898 (2018).
14. S. Javaid<sup>†</sup>, **C. W. Myung**<sup>†</sup>, J. Yun, G. Lee & K. S. Kim (<sup>†</sup>equally contributed), Organic cation steered interfacial electron transfer within organic–inorganic perovskite solar cells. *J. Mater. Chem. A* **6**, 4305 (2018).
15. T. Yoon<sup>†</sup>, G.-H. Kim<sup>†</sup>, **C. W. Myung**<sup>†</sup>, S. Kajal, J. Jeong, J. Y. Kim & K. S. Kim (<sup>†</sup>equally contributed), Ambient-stable cubic-phase hybrid perovskite reaching the shockley-queisser fill factor limit via hydrazinium chloride additive-assisted process. *ACS Appl. Energy Mater.* **1**, 5865-5871 (2018).
16. Y. Park<sup>†</sup>, Y. S. Kim<sup>†</sup>, **C. W. Myung**<sup>†</sup>, R. A. Taylor, C. C. S. Chan, B. P. L. Reid, T. J. Puchtler, R. J. Nicholas, L. T. Singh, G. Lee, C.-C. Hwang, C.-Y. Park & K. S. Kim (<sup>†</sup>equally contributed), Two-dimensional excitonic photoluminescence in graphene on a Cu surface. *ACS Nano* **11**, 3207-3212 (2017).
17. M. R. Rezapour<sup>†</sup>, **C. W. Myung**<sup>†</sup>, J. Yun, A. Ghassami, N. Li, S. U. Yu, A. Hajibabaei, Y. Park & K. S. Kim (<sup>†</sup>equally contributed) Graphene and graphene analogs toward optical, electronic, spintronic, green-chemical, energy-material, sensing, and medical applications. *ACS Appl. Mater. Interfaces* **9**, 24393-24406 (2017).
18. H. J. Jang, J. Y. Maeng, Y. J. Kim, I. Yoon, **C. W. Myung**, C. K. Rhee, Y. Sohn, Electrocatalytic CO<sub>2</sub> reduction reaction over group 15 bismuth and antimony film electrodes: What makes difference? *Journal of CO<sub>2</sub> Utilization* **64**, 102202 (2022).
19. A. Jana, **C. W. Myung**, V. G. Sree & Kwang S. Kim, Upconversion and multiexciton generation in organic Mn(II) complex boost the quantum yield to > 100%. *Mater. Chem. Front.* **6**, 3102-3114 (2022).
20. A. Hajibabaei, **C. W. Myung**, & K. S. Kim, Sparse Gaussian process potentials: Application to lithium diffusivity in superionic conducting solid electrolytes. *Phys. Rev. B* **103**, 214102 (2021).
21. S. Pourasad, A. Hajibabaei, **C. W. Myung** & K. S. Kim, Two Liquid–Liquid Phase Transitions in Confined Water Nanofilms. *J. Phys. Chem. Lett.* **12**, 4786 (2021).
22. S. Kajal, J. Kim, Y. S. Shin, A. N. Singh, **C. W. Myung**, J. Y. Kim & K. S. Kim Unfolding the Influence of Metal Doping on Properties of CsPbI<sub>3</sub> Perovskite. *Small Methods* 2000296 (2020).
23. V. Gladkikh, D. Y. Kim, A. Hajibabaei, A. Jana, **C. W. Myung**, K. S. Kim, Machine Learning the Band Gaps of ABX<sub>3</sub> Perovskites from Elemental Properties. *J. Phys. Chem. C* **124**, 8905-8918 (2020).
24. S. Kajal, G.-H. Kim, **C. W. Myung**, J. Kim, Y. Shin, J. Jeong, A. Jana, J. Y. Kim, Kwang S. Kim, A thermally stable, barium-stabilized  $\alpha$ -CsPbI<sub>3</sub> perovskite for optoelectronic devices. *J. Mater. Chem. A* **7**, 21740-21746 (2019).

25. J. N. Tiwari, A. M. Harzandi, M. Ha, S. Sultan, **C. W. Myung**, H. J. Park, D. Y. Kim, P. Thangavel, A. N. Singh, P. Sharma, S. S. Chandrasekaran, F. Salehnia, J.-W. Jang, H. S. Shin, Z. Lee & Kwang S. Kim, High-performance hydrogen evolution by Ru single-atoms and nitrided-Ru nanoparticles implanted on N-doped graphitic sheet. *Adv. Ener. Mater.* **9**, 1900931 (2019).
26. S. Sultan, J. N. Tiwari, A. N. Singh, S. Zhumagali, M. Ha, **C. W. Myung**, P. Thangavel, K. S. Kim, Single Atoms and Clusters Based Nano-Materials for Hydrogen Evolution, Oxygen Evolution Reactions, and full Water Splitting. *Adv. Ener. Mater.* **9**, 1900624 (2019).
27. J. N. Tiwari, S. Sultan, **C. W. Myung**, T. Yoon, N. Li, M. Ha, A. M. Harzandi, H. J. Park, D. Y. Kim, S. S. Chandrasekaran, W. G. Lee, V. Vij, H. Kang, T. J. Shin, H. S. Shin, G. Lee, Z. Lee & K. S. Kim, Multicomponent electrocatalyst with ultralow Pt loading and high hydrogen evolution activity. *Nat. Energy* **3**, 773–782 (2018).
28. S. Javaid, **C. W. Myung**, B. Rakshit, K. S. Kim & G. Lee, A highly hydrophobic fluorographene-based system as an interlayer for electron transport in organic–inorganic perovskite solar cells. *J. Mater. Chem. A* **6**, 18635-18640 (2018).
29. B. Park, K. Kim, J. Park, H. Lim, P. T. Lanh, A. Jang, C. Hyun, **C. W. Myung**, S. Park, J. W. Kim, K. S. Kim, H. S. Shin, G. Lee, S. H. Kim, C. E. Park & J. K. Kim, Anomalous Ambipolar Transport of Organic Semiconducting Crystals via Control of Molecular Packing Structures. *ACS Appl. Mater. Interfaces* **9**, 27839-27846 (2017).
30. C. Hyun, J. Yun, W. J. Cho, **C. W. Myung**, J. Park, G. Lee, Z. Lee, K. Kim & K. S. Kim Graphene edges and beyond: temperature driven structures and electromagnetic properties. *ACS Nano* **9**, 4669-4674 (2015).

## Funding

- National Research Foundation of Korea, 우수신진연구 (NRF-2022R1C1C1010605) “Understanding redox process in lithium ion battery using multiple electronic states machine learning molecular dynamics (다중전자상태 머신러닝 분자동역학 개발을 통한 리튬이온 배터리 물질 내 산화/환원 현상 연구)” 2022-03-01 to 2027-02-28 (460,005,000 KRW)
- National Research Foundation of Korea, 박사후국외연수, “Emergent phases and nucleation of superionic water using machine learning nuclei exchange path integral molecular dynamics (머신러닝 기반 핵교환 경로적분 동역학을 활용한 초이온성 물 상태 및 핵생성 연구)” 2020-09-01 to 2021-11-30 (45,000,000 KRW)

## Conference & Seminar

1. **Invited talk** MOF & Beyond, 2022/12/14-17, Jeju island, Korea, “Development of Next Generation Sparse Gaussian Process Regression (SGPR) Machine Learning Potential”
2. **Invited talk** ENGE 2022, 2022/11/7, Jeju island, Korea, “Anharmonicity-Driven Rashba Cohelical Excitons Break Quantum Efficiency Limitation”
3. **Invited talk** Workshop on Computational Design of Catalysts, 2022/11/1, Jeonbuk National University, Jeonju, Korea, “Next Generation Machine Learning Potential and its Applications to Energy Materials”
4. **Contribution talk** Psi-k 2022, EPFL, Lausanne, Switzerland, 2022/08/23 “Prediction of a supersolid phase in high-pressure deuterium”
5. **Invited talk** Korean Chemical Society, Physical Chemistry Division Meeting, 2022/02/18, Yonsei University “How to be a solid yet more fluid than a fluid: Prediction of a supersolid phase in high-pressure deuterium”
6. **Invited talk** International Symposium on Materials Chemistry, 2021/11/11, Online (Zoom), “Machine learning design of energy materials: challenges and opportunities”
7. **Invited talk** 2021 KOREA-VIETNAM SCIENCE & ENGINEERING SYMPOSIUM, 2021/09/16-17, Online (Zoom), “Computational design of single-atom and nanocluster catalysts at first-principles level”
8. **Contribution poster** The International Symposium on Ab Initio Electron Dynamics Simulations (AIEDS18), 2018/11/14-16, Tsukuba, Japan, “X-ray Absorption Fine Spectra of Single Pt on N-doped Coronene”.
9. **Contribution poster** PITP2016, 2016/05/30-06/09, Sherbrooke, Canada, “Non-equilibrium Kondo effect in nanoscale quantum dots using NCA and beyond”.
10. **Contribution poster** JMC15, 2015/08/22-26, Université de Bordeaux, Bordeaux, France, “Non-equilibrium transport of two sites anderson impurity model with vertex corrections”.
11. **Contribution poster** IUPAC, 2015/08/07-13, Bexco, Busan, Korea, “Electronic and magnetic properties of defected MoS<sub>2</sub> nanotubes: A first-principle study”.

## Patent (KR)

1. 10-2388382 (등록일자: 2022년 4월 14일), 물 분해를 위한 Ru 촉매, 이를 포함한 물 분해 장치 및 이의 제조 방법
2. 10-2021-0049699 (공개일자: 2021년 5월 6일), 수소 발생을 위한 다중 복합 화합물, 이를 포함한 수소 발생 장치 및 이의 제조 방법
3. 10-1518745 (2015년 5월 1일), 생의학용 플라즈마 발생을 위한 증폭기 출력의 안정화 피드백 회로

## Reference

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