Curriculum Vitae

Personal Information

Name:	Chang Woo Myung
Nationality:	Korea, Republic of
Born:	14 February 1989 (Seoul, Korea)
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Researcher ID:	V-2298-2018
Google Scholar:	https://scholar.google.com/citations?user=YqlmqKYAAAAJ&hl=en
Status:	Married
Language:	Korean(vernacular), English(fluent) and Italian(Livello A1 del Quadro Comune Europeo)

Professional experience

- **01/12/2020-**
  Postdoctoral Fellow of National Research Foundation of Korea,
  University of Cambridge, United Kingdom
  Research Group: Prof. Angelos Michaelides
- **01/12/2019-30/11/2020**
  Postdoctoral Researcher, ETH Zürich & Università della Svizzera italiana (USI), Switzerland
  Research Group: Prof. Michele Parrinello
- **13/02/2019-30/11/2019**
  Postdoctoral Researcher, Ulsan National Institute of Sci. and Tech. (UNIST), Korea
  Research Group: Prof. Kwang S. Kim

Education

- **01/09/2014-12/02/2019**
  PhD, Department of Chemistry, Ulsan National Institute of Sci. and Tech. (UNIST)
  Supervisor: Prof. Kwang S. Kim
  Dissertation title: "*First-Principles calculation of energy materials*"
- **01/09/2012-08/08/2014**
  MS, Pohang Univ. of Sci. and Tech. (POSTECH)
- **01/03/2007-10/08/2012**
  BS, Pohang Univ. of Sci. and Tech. (POSTECH)

Unpublished Works (under review)

1. **C. W. Myung**, B. Hirshberg & M. Parrinello, Anomalous deuterium quantum crystal under pressure. (to be submitted) (2020).
   Role: As a first author, I developed the state-of-the-art Bosonic path integral NPT molecular dynamics simulation and identified significant nuclear quantum effects in high-pressure hydrogen/deuterium solid through machine learning *ab initio* potential.
   # of citations: 0

2. **C. W. Myung** & K. S. Kim, Anharmonicity-driven exciton fine structure transition between dark singlet to bright Rashba spin-orbit co-helical exciton in lead halide perovskites. *Adv. Mater.* (under review) arXiv:2004.02329 (2020).
   Role: As a first author, I revealed the mechanism behind the high internal quantum efficiency of lead halide perovskite light-emitting diodes using DFT and the Bethe-Salpeter equations. Inversion-breaking anharmonicity, sizeable spin-orbit coupling, and co-helicity of spin states give rise to a favourable exciton fine structure for efficient light emission.

 # *of citations:* 0

3. A. Hajibabaei, **C. W. Myung**, & K. S. Kim, Towards Universal Sparse Gaussian Process Potentials: Application to Lithium Diffusivity in Superionic Conducting Solid Electrolytes. *Phys. Rev. Lett.* (under review) (2020).
   Role: As a co-author, I contributed to developing the sparse Gaussian process for *ab initio* machine learning potential, which is faster than the conventional Gaussian process.
   # *of citations:* 0

4. S. Pourasad, A. Hajibabaei, **C. W. Myung** & K. S. Kim, Confined water reveals a new story about liquid–liquid phase transition. *Sci. Adv.* (under review) arXiv:2006.15295 (2020).
   Role: As a co-author, I contributed to deriving a Landau theory based on many-body interactions and explained a hidden "mid-density" phase of supercooled water at 2D confined environment.
   # *of citations:* 0

Publications (without self-citation)

5. J. Kim, Kwang S. Kim*, & **C. W. Myung***(*co-corresponding author) Superb band alignment, defect tolerance, and carrier injection property of SnO_2 electron transport layer for perovskite solar cells. *npj Computational Mater.* **6**, 100 (2020).
   Role: As a co-corresponding author, I elucidated the electron extraction and defect states at the SnO_2/$MAPbI_3$ interface using DFT calculations.
   # *of citations:* 0

6. 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 $CsPbI_3$ Perovskite. *Small Methods* 2000296 (2020).
   Role: As a co-author, I explained the metal-doping effect on $CsPbI_3$ using DFT calculations.
   # *of citations:* 0

7. V. Gladkikh, D. Y. Kim, A. Hajibabaei, A. Jana, **C. W. Myung**, K. S. Kim, Machine Learning the Band Gaps of ABX_3 Perovskites from Elemental Properties. *J. Phys. Chem. C* **124**, 8905-8918 (2020).
   Role: As a co-author, I contributed to the machine learning model of bandgap predictions on cubic perovskite materials.
   # *of citations:* 4

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), Hydrogen evolution by immiscible bi-metallic single-atoms and nanoparticles embedded in N-doped graphitic matrix. *Applied Catalysis B: Environmental* **270**, 118896 (2020).
   Role: As a co-corresponding author, I performed the density functional theory calculations of Cu/Ru/N-doped graphitic carbon catalysts for Gibbs free energy and band structures (conductivity). I also calculated the X-ray absorption spectra using the restricted open-shell configuration interactions simulations.
   # *of citations:* 2

9. Y. Park†, A. Jana†, **C. W. Myung**†, T. S. Yoon, T. J. Puchtler, C. C. Kocher, R. A. Taylor & K. S. Kim (†equally contributed). Large enhancement of optical quantum efficiency of $MAPbBr_3$ by encapsulating graphene. *Nano Research* **13**, 932–938 (2020).
   Role: As a co-first author, I performed the density functional theory calculations of $MAPbI_3$/graphene interfaces with various defect states to explain the mechanism behind the experimental observations of optical quantum efficiency enhancements.
   # *of citations:* 1

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 $Fe_3Co(PO_4)_4$ designed with computation-aid. *Nat. Commun.* **10**, 5195 (2019).
    Role: As a co-corresponding author, I computationally designed the highly efficient Fe/Co-based oxygen evolution catalysts using the density functional theory calculations.
    # *of citations:* 14

11. 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 α-$CsPbI_3$ perovskite solar cells. *J. Mater. Chem. A* **7**, 21740-21746 (2019).
Role: As a co-author, I explained the stabilizing effect of Ba using the density functional theory calculations.
 # *of citations:* 5

12. 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).
Role: As a co-author, I calculated the electronic structures of Ru/N-doped graphene catalysts.
 # *of citations:* 28

13. 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).
Role: As a co-author, I contributed a review on theoretical mechanisms of water-splitting catalysts.
 # *of citations:* 76

14. T. Yoon[†], G.-H. Kim[†], **C. W. Myung**[†], S. Kajal, J. Jeong, J. Y. Kim & K. S. Kim ([†]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).
Role: As a co-first author, based on the prediction of my work 12, I provided the mechanism behind the increase in the solar cell efficiency of lead halide perovskite MA/HZPbI_3 using the density functional theory and many-body perturbation theory.
 # *of citations:* 5

15. 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).
Role: As a co-author and as the main author of theory part, I provided a crucial theoretical mechanism behind the hydrogen evolution reaction (HER) of single atom plus nanoparticle Pt on N-doped graphite carbon using the density functional theory calculations. This was the best HER performance at that time. And now this strategy is widely used by the community for designing highly efficient single-atom catalysts.
 # *of citations:* 117

16. **C. W. Myung**, G. Lee & K. S. Kim, La-doped $BaSnO_3$ electron transport layer for perovskite solar cells, *J. Mater. Chem. A* **6**, 23071-23077 (2018).
Role: As a first author, I studied the La-doped $BaSnO_3$/MAPbI3 interface, revealing the effect of La-doping on the band alignment.
 # *of citations:* 8

17. S. Javaid, **C. W. Myung**, B. Rakshit, K. S. Kim & G. Lee, 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).
Role: As a co-author, I contributed a theoretical calculation of fluorographene-based lead halide perovskite solar cell system using DFT.
 # *of citations:* 10

18. **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).
Role: As a first author, I elucidated a large Rashba-Dresselhaus effect at the interface of lead halide perovskites and discussed a crucial role of Rashba-Dresselhaus effect on the electron extraction mechanism.
 # *of citations:* 13

19. **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).

Role: **As a first author**, I elucidated the effect of A-site cations on the Fröhlich polarons in lead halide perovskites using the many-body theory and DFT calculations. I also suggested novel A-site cations for the better solar cell efficiency.
 # *of citations:* 17

20. S. Javaid[†], **C. W. Myung[†]**, J. Yun, G. Lee & K. S. Kim ([†]equally contributed), Organic cation steered interfacial electron transfer within organic–inorganic perovskite solar cells. *J. Mater. Chem. A* **6**,4305 (2018).
Role: **As a co-first author**, I studied the effect of hydrogen bonding at the TiO_2/$MAPbI_3$ using *ab initio* molecular dynamics.
 # *of citations:* 3

21. Y. Park[†], Y. S. Kim[†], **C. W. Myung[†]**, 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 ([†]equally contributed), Two-dimensional excitonic photoluminescence in graphene on a Cu surface. *ACS Nano* **11**, 3207-3212 (2017).
Role: **As a co-first author**, I explained anomalous photoluminescence at ~400 nm from a Cu/graphene system using the density functional theory calculations.
 # *of citations:* 6

22. M. R. Rezapour[†], **C. W. Myung[†]**, J. Yun, A. Ghassami, N. Li, S. U. Yu, A. Hajibabaei, Y. Park & K. S. Kim ([†]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).
Role: **As a co-first author**, I contributed a review paper on graphene-based optoelectronics, spintronics and energy-materials applications.
 # *of citations:* 26

23. 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).
Role: As a co-author, I contributed to the understanding of the band structure of pentacene molecular crystal using DFT calculations.
 # *of citations:* 4

24. 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).
Role: As a co-author, I contributed a perspective paper on the present understanding, issues, and future challenges faced in the field of graphene-edge-based nanodevices.
 # *of citations:* 19

Presentations

- **November 2018, Ab initio Electron Dynamics Simulations (Tsukuba, Japan)** X-ray Absorption Fine Spectra of Single Pt on N-doped Coronene.
- **June 2016, International Summer School on Computational Quantum Materials (Sherbrooke, Canada)** Non-equilibrium Kondo effect in nanoscale quantum dots using NCA and beyond.
- **August 2015, IUPAC-2015 (Busan, Korea)** Electronic and magnetic properties of defected MoS_2 nanotubes: A first-principle study.

Prizes and Awards

- Postdoctoral fellow of National Research Foundation of Korea (01/09/20-30/11/21).
- Best paper, Korea Institute of Science and Technology (2019).
- Best presentation, Winter school of statistical physics, Korea Institute for Advanced Study (2018).

Funding

- Nurturing Next-generation Researchers 2020 “Emergent phases and nucleation of superionic water using machine learning nuclei exchange path integral molecular dynamics”, National Research Foundation of Korea. 12/2020 to 11/2021.
- European Union Grant No. ERC-2014-AdG-670227/VARMET “Variational Metadynamics”. 12/2019 to 11/2020.
- Korea Institute of Science and Technology Information Creative Research (KSC-2019-CRE-0248) “Exciton-Phonon Interactions and Rashba Effect in Lead Halide Perovskites” 01/2020 to 11/2020.
- Korea Institute of Science and Technology Information Creative Research (KSC-2019-CRE-0139) “Fast and accurate large scale ab initio molecular dynamics simulations for free energy calculations using machine learning.” 10/2019 to 09/2020.
- Korea Institute of Science and Technology Information Creative Research (KSC-2018-CRE-0071) “Mechanism for multi-exciton generations in high spin transition metal zero dimensional crystals: beyond the Shockley-Quiesser limit.” 12/2018 to 12/2019.
- National Honor Scientist Program (2010-0020414), National Research Foundation of Korea “Innovative nanomaterials and nanodevices” 09/2014 to 11/2019.

Supervising and mentoring

I have supervised 3 PhD students in Prof. Kwang S. Kim’s group (12/02/2019-30/11/2019) by publishing three peer-reviewed journals **as a corresponding author**.

- *Nat. Commun.* **10**, 5195 (2019): Water splitting is the essential electrochemical reaction in hydrogen production. And the oxygen evolution reaction (OER) is most challenging reaction step because the understanding of the microscopic OER mechanism is hard, and the improvement of the electrocatalytic performance (over-potential and turn-over frequency) of the OER is arduous. In this work, **I supervised and guided 2 PhD students for the extensive DFT calculations of novel phosphate-based Fe catalyst to uncover the structure of nanoparticle and electronic origin of high OER performance.**

- *Applied Catalysis B: Environmental* **270**, 118896 (2020): High-performance hydrogen evolution Cu/Ru bi-metallic single atom electrocatalyst was synthesized and analyzed for the first time. Immiscible bi-metallic synthesis is advantageous for boosting the reactivity and for high stability because of immiscibility-driven aggregation-blocked single-/nano-particles. In this work, **I supervised and guided 1 PhD student to prove the structure and immiscibility of Ru-Cu atoms (DFT/ROCIS X-ray absorption spectroscopy, DFT calculations) and to explain the origin of high over-potential and turn-over frequency of Cu/Ru catalyst.**

- *npj Computational Mater.* **6**, 100 (2020): Lead halide perovskite solar cell (power conversion efficiency of 25.2 %, August 2020) is one of the promising next-generation solar cell materials, which poses a significant advantage in large-scale thin-film manufacturing, easy synthesis, defect-tolerance, easy bandgap tuning and high mobility. Recently, the importance of the electron transport layer (ETL) has been recognized, and extensive research on ETL is on the way. Among many ETL materials, SnO_2 is a promising ETL material because of its chemical stability, UV-resistance, superior band alignment, high charge extraction, and less photocatalytic activity. In this work, **I supervised and guided 1 PhD student for elucidating the electronic/atomistic origin of efficient electron extraction and defect tolerance of the SnO_2/$MAPbI_3$ interface.**