Miran Ha

Postdoctoral Researcher
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Research Interests

- Computational Catalysis
- Materials Design through High-Throughput Density Functional Theory Calculations

Position

- ***UNIST***, Postdoctoral researcher (Prof. Geunsik Lee, Prof. Kwang S. Kim) Mar. 2021 ~ Present
- ***UNIST***, Graduate Research assistant (Prof. Kwang S. Kim) Apr. 2015 ~ Feb. 2021

Education

- ***UNIST***, Integrated M.S. & Ph.D in Chemical Engineering (Prof. Chunggi Baig) Mar. 2014 ~ Feb. 2021
  Thesis: First-Principles Calculation for Surface Chemistry of Electrocatalysts
- ***UNIST***, B.S. in Chemical Engineering Mar. 2010 ~ Feb. 2014

Honors & Awards

- Outstanding Paper Award, Korea Institute of Science and Technology Information (KISTI), Korea 2019
- The 27th Humantech Paper Award, Bronze Prize, Samsung, Korea (Co-author) 2021
- The 26th Humantech Paper Award, Participation Prize, Samsung, Korea (Co-author) 2020

Funding

- Basic Science Research Program, *NRF* (140M KRW) Jun. 2021 ~ May. 2023
- R&D Innovation Support Program Based on HPC, *KISTI* (25M KRW worth) Jan. 2022 ~ Dec. 2022
- R&D Innovation Support Program Based on HPC, *KISTI* (15M KRW worth) May. 2020 ~ Apr. 2021

Publications

Total Publications: 20 († = Co-first Author)

1. **M. Ha**†, D. Y. Kim†, M. Umer†, V. Gladkikh, C. W. Myung*, K. S. Kim*, “Tuning metal single atoms embedded in N x C y moieties toward high-performance electrocatalysis”, ***Energy & Environmental Science***, 14, 3455 (2021)
2. S. Sultan†, M. H. Diorizky†, **M. Ha**†, J. N. Tiwari, H. Choi, N. K. Dang, P. Thangavel, J. H. Lee, H. Y. Jeong, H. S. Shin*, Y. Kwon*, K. S. Kim*, “Modulation of Cu and Rh single-atoms and nanoparticles for high-performance hydrogen evolution activity in acidic media”, ***Journal of Materials Chemistry A***, 9, 10326 (2021)
3. D. Y. Kim, **M. Ha**, K. S. Kim*, “Universal Screening Strategy for Accelerated Design of Superior Oxygen Evolution/Reduction Electrocatalysts”, ***Journal of Materials Chemistry A***, 9, 3511 (2021)

4. A. Hajibabaei, **M. Ha**, S. Pourasad, J. Kim, K. S. Kim*, “Machine Learning of First-Principles Force-Fields for Alkane and Polyene Hydrocarbons”, ***Journal of Physical Chemistry A***, 125, 9414 (2021)
5. R. Anand, A. S. Nissimagoudar, M. Umer, **M. Ha**, M. Zafari, S. Umer, G. Lee*, K. S. Kim*, “Late Transition Metal Doped MXenes Showing Superb Bifunctional Electrocatalytic Activities for Water Splitting via Distinctive Mechanistic Pathways”, ***Advanced Energy Materials***, In press (2021) (doi: 10.1002/aenm.202102388)
6. S. Kim, J. U. Hong, **M. Ha**, S. M. Noh, “Dual-curable isocyanate crosslinking agents blocked by methacrylate-functionalized pyrazoles with lower curing temperature”, ***Progress of Organic Coatings***, 161, 106501 (2021)
7. Y. S. Choi, S. E. Kim, **M. R. Ha**, J. C. Kim, H.-J. Paik*, S.-H. Lee*, Y. I. Park*, “Metal acetylacetonate as a radical initiator and catalyst for polyurethane in dual-curing reaction at low temperature”, ***Progress of Organic Coatings***, 151, 105926 (2021)
8. Y.-G. June, K. I. Jung, T. H. Lee, **M. Ha**, S. M. Noh*, H. W. Jung*, “Effect of isocyanate crosslinkers blocked with amine derivatives on rheological and crosslinking characteristics of automotive clearcoats”, ***Korea-Australia Rheology Journal***, 33, 37 (2021)
9. M. Harzandi†, S. Shadman†, **M. Ha**†, C. W. Myung*, D. Y. Kim*, H. J. Park, S. Sultan, W.-S.Noh, W. Lee, P. Thangavel, W. J. Byun, S.-H. Lee, J. N. Tiwari, T. J. Shin, J.-H. Park, Z. Lee, J. S. Lee, K. S. Kim*, "Immiscible bi-metal single-atoms driven synthesis of electrocatalysts having superb mass-activity and durability", ***Applied Catalysis B, Environmental***, 270, 118896 (2020)
10. P. Thangavel, **M. Ha**, S. Kumaraguru, A. Meena, A. N. Singh, A. M. Harzandi, K. S. Kim*, “Graphene-nanoplatelets-supported NiFe-MOF: high-efficiency and ultra-stable oxygen electrodes for sustained alkaline anion exchange membrane water electrolysis”, ***Energy & Environmental Science***, 13, 3447 (2020)
11. H. Jin, S. Sultan, **M. Ha**, J. N. Tiwari, M. G. Kim, K. S. Kim*, “Simple and Scalable Mechanochemical Synthesis of Noble Metal Catalysts with Single Atoms toward Highly Efficient Hydrogen Evolution”, ***Advanced Functional materials***, 30, 2000531 (2020)
12. M. Choi, M. G. Kim, K. I. Jung, T. H. Lee, **M. Ha**, W. Hyung, H. W. Jung, S. M. Noh, “Reactivity and Curing Efficiency of Isocyanate Cross-Linkers with Imidazole-Based Blocking Agents for Low-Temperature Curing of Automotive Clearcoats”, ***Coatings***, 10, 974 (2020)
13. S. Sultan†, **M. Ha**†, D. Y. Kim†, J. N. Tiwari*, C. W. Myung*, A. Meena, T. J. Shin, K. H. Chae, K. S. Kim*, "Superb water splitting activity of the electrocatalyst $Fe_3Co(PO_4)_4$ designed with computation aid", ***Nature Communications***, 10, 5195 (2019)
14. 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, K. S. Kim*, "High-Performance Hydrogen Evolution by Ru Single Atoms and Nitrided-Ru Nanoparticles Implanted on N-Doped Graphitic Sheet", ***Advanced Energy Materials***, 9, 1900931 (2019) (Highlighted as a Front cover paper)
15. A. Meena, **M. Ha***, S. S. Chandrasekaran, S. Sultan, P. Thangavel, A. M. Harzandi, B. Singh, J. N. Tiwari*, K. S. Kim*, "Pt-like hydrogen evolution on a V_2O_5/$Ni(OH)_2$ electrocatalyst", ***Journal of Materials Chemistry A***, 7, 15794-15800 (2019)
16. 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 Nanomaterials for Hydrogen Evolution, Oxygen Evolution Reactions, and Full Water Splitting", ***Advanced Energy Materials***, 9, 1900624 (2019)
17. T. Yoon†, G. Song†, A. M. Harzandi, **M. Ha**, S. Choi, S. Shadman, J. Ryu, T. Bok, S. Park*, K. S. Kim*, "Intramolecular deformation of zeotype-borogermanate toward a three-dimensional porous germanium anode for high-rate lithium storage", ***Journal of Materials Chemistry A***, 6, 15961-15967 (2018)
18. 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", ***Nature Energy***, 3, 773-782 (2018)

19. **M. Ha**†, D. Y. Kim†, N. Li, J. M. L. Madridejos, I. K. Park, I. S. Youn, J. Lee, C. Baig, M. Filatov, S. K. Min*, G. Lee*, K. S. Kim*, "Adsorption of Carbon Tetrahalides on Coronene and Graphene", ***Journal of Physical Chemistry C***, 121, 14968-14974 (2017)
20. D. Y. Kim, J. M. L. Madridejos, **M. Ha**, J.-H. Kim, D. C. M. Yang, C. Baig, K. S. Kim*, "Size-dependent conformational change in halogen-π interaction: from benzene to graphene", ***Chemical Communications***, 53, 6140-6143 (2017)