Curriculum Vitae

Hyeyoung Shin

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PROFESSIONAL EXPERIENCE

09.2023 – **Present** **Associate Professor**
Graduate School of Energy Science and Technology, CNU, Republic of Korea

09.2019 – 08.2023 **Assistant Professor**
Graduate School of Energy Science and Technology, CNU, Republic of Korea

03.2019 – 08.2019 **Senior Engineer**
Samsung Electronics, Republic of Korea

12.2016 – 12.2018 **Postdoctoral Scholar**
Division of Chemistry and Chemical Engineering, California Institute of Technology, United States

(Advisor: Prof. William A. Goddard III)

09.2016 – 12.2016 **Postdoctoral Scholar**
Applied Science Research Institute, KAIST, Republic of Korea

EDUCATION

08.2016 **Ph.D.** Graduate School of EEWS (Energy, Environment, Water and Sustainability), KAIST, Daejeon, Republic of Korea

(Advisor: Prof. Hyungjun Kim)
Thesis: *Multiscale materials modelling and design for heterogeneous catalysts applications*

02.2013 **M.S.** Graduate School of EEWS, KAIST, Daejeon, Republic of Korea
Thesis: *Development of first-principle based methods for predicting the structures and properties of solvated polymers*

02.2011 **B.S.** Department of Chemical Engineering, Hanyang University, Ansan, Republic of Korea

RESEARCH INTERESTS

- Materials for energy and environmental applications (Fuel cell, CO_2 conversion, water splitting)
- Interfacial phenomenon on materials: spillover, kinetics, electrical double layer

- *In-silico* design of materials/high-throughput screening for discovery of novel materials
- Electrical, physical and chemical properties of materials
  Development of improved techniques for fundamental understanding on materials

EXPERTISE

Multi-scale Simulation

- *Classical/ReaxFF/Tersoff Molecular Dynamics*: Large-scale Atomic Modeling Massively Parallelized Simulation (LAMMPS)
- *Density Functional Theory*: Vienna Ab-initio Software Package (VASP), Jaguar, jDFTx, CRYSTAL
- *Grand Canonical Monte Carlo* (GCMC): Materials Studio, Cerius2
- Development of first-principles based force field for molecular dynamics/Monte Carlo simulations
- Development of methods for predicting the structures of solvated polymers
  ('Scaled Effective Solvent method' is published in *J. Phys. Chem. B* **117**, 916 (2013) and is now available in *Materials Science Suite* program of Schrödinger company)
- Visual Molecular Dynamics (VMD), Visualization for Electronic and STructural Analysis (VESTA), p4vasp, Matlab, Materials Studio

AWARDS AND HONORS

- Selected as 2017 Rising Researcher in Korea - The Korean Academy of Science and Technology
- Winner of Schrödinger's 2016 Excellence in Materials Science Applications Publication Contest
- Dissertation of the Year (2016) by S-OIL Science Prodigy and Culture Foundation – Grand (1^{st}) prize in Chemistry division
- 22^{nd} Samsung HumanTech Paper Award (2016) – Silver (2^{nd}) prize in Basic Science & Technology division
- 22^{nd} Samsung HumanTech Paper Award (2016) – Participation (4^{th}) prize in Energy & Environment division
- Deputy Premier Award (2015) from the Ministry of Education, Korea

PUBLICATIONS (SCIE)

1. W.-G. Lim+, H. N. Truong+, J.-Y. Jeong, D. Kim, L. S. Oh, C. Jo, C. Kim, H. J. Kim, S. M. Choi, **H. Shin***, S. Lee*, E. Lim*, Toward Feasible Single Atom-based Hydrogen Evolution Electrocatalysts via Artificial Ensemble Sites for Anion Exchange Membrane Water Electrolyzer, *Applied Catalysis B: Environmental*, 343, 123568 (2024)
2. C. Lim, D. Kim, M. Kim, H. Yun, D. Shin, Y. J. Hwang, **H. Shin**, K. Yong*, Effect of Sulfur-Derived Solid Electrolyte Interphase on Li-mediated Nitrogen Reduction, *ACS Energy Lett.*, **8**, 4875 (2023)
3. S. Jo, S. Im, S. Weon, **H. Shin***, J. Lim*, Reduced TiO_2 Nanotube Arrays as Environmental Catalysts that Enable Advanced Oxidation Processes: A Mini Review, *Chem. Eng. J.*, **477**, 147031 (2023) **-Invited for a special issue on "Emerging Trends on the Role of AOPs in Water Reuse Applications"**

4. H. Lee, W. A. Goddard III, J. Cha, W. J. Choi*, S. H. Noh*, **H. Shin***, H. Kim*, Functional Group-Dependent Proton Conductivity of Phosphoric Acid-Doped Ion-Pair Coordinated Polymer Electrolytes: A Molecular Dynamics Study, *J. Phys. Chem. B*, **127**, 8993 (2023)
5. J. Park, M. Jeong, Y. J. Cho, K. J. Kim, T. B. Tai, **H. Shin**, J. C. Lim, H. S. Chang*, Investigation of tetrakis(ethylmethylamido)hafnium adsorption mechanism in initial growth of atomic layer deposited-HfO_2 thin films on H-/OH-terminated Si (100) surfaces, *J. Vac. Sci. Technol. B*, **41**, 062801 (2023)
6. R. S. Kanase, G. M. Zewdie, M. Arunachalam, J. Badiger, S. A. Sayed, K.-S. Ahn, J.-S. Ha, U. Sim, **H. Shin***, S. H. Kang*, Surface Engineering of ZnO Electrocatalyst by N Doping Towards Electrochemical CO_2 Reduction, *J. Energy Chem.*, **88**, 71 (2023)
7. H. S. Moon, B. Song, J. Jeon, T.-H. Lai, Y.-P. Chang, Y.-D. Lin, J. K. Park, Y.-G. Lin, Y.-J. Hsu, **H. Shin**, Y. Yun, K. Yong*, Atomically isolated copper on titanium dioxide for ammonia photosynthesis via nitrate reduction with unprecedently high apparent quantum yield, *Applied Catalysis B: Environmental*, **15**, 123185 (2023)
8. Y. A. Lee+, K. Y. Jang+, J. Yoo+, K. Yim, W. Jung, K. Jung, C. Yoo, Y. Cho, J. Lee, M. H. Ryu, **H. Shin*,** K. Lee*, H. Yoon*, Three-Dimensional Flower-like MoS_2 Nanosheets Grown on Graphite as High-Performance Anode Materials for Fast-Charging Lithium-Ion Batteries, *Materials*, **16**, 4016 (2023) **-highlighted as a front cover**
9. Y. Jung+, **H. Shin+**, S.-W. Baek, T. B. Tai, B. Scheffel, O. Ouellette, M. Biondi, S. Hoogland, A. F. P. Garcia, E. Sargent*, Near-Unity Broadband Quantum Efficiency Enabled by Colloidal Quantum Dot/Mixed-Organic Heterojunction, *ACS Energy Lett.*, **8**, 2331 (2023) **(co-1st Author)**
10. M. S. Kim, H. Y. Yoo, G. E. Choi, S. Jo, **H. Shin**, J. Lim*, Visible Light Photocatalysis of TiO_2 Complexed with Albumin via a Ligand-to-Metal Charge Transfer (LMCT) Pathway, *J. Phys. Chem. C* **127**, 5408 (2023)
11. T. B. Tai, J. Son, **H. Shin***, A theoretical study of the atomic layer deposition of HfO_2 on Si(100) surfaces using tetrakis(ethylmethylamino) hafnium and water. *Appl. Surf. Sci.* **612**, 155702 (2023)
12. H. M. Choi, S. J. Jun, J. Lee, M.-H. Ryu, **H. Shin***, K.-N. Jung*, UV-cured Polymer Solid Electrolyte Reinforced using a Ceramic-Polymer Composite Layer for Stable Solid-State Li Metal Batteries. *J. Electrochem. Sci. Technol.* **14**, 85 (2023)
13. W. Jung, J. Jeong, Y. Chae, W. H. Lee, Y.-J. Ko, K. H. Chae, H.-S. Oh, U. Lee, D. K. Lee, B. K. Min, **H. Shin***, Y. J. Hwang*, D. H. Won*, Synergistic CuPd bimetallic electrocatalyst for ammonia production from electrochemical nitrate reaction. *J. Mater. Chem. A* **10**, 23760 (2022)
14. D. Shin, H. Choi, J. An, C-H. Choi, C.-H. Sohn, **H. Shin***, H. Kim*, Enhanced Electroreduction of CO_2 by Ni−N−C Catalysts from the Interplay Between Valency and Local Coordination Symmetry. *J. Mater. Chem.* A **10**, 22523 (2022)
15. H. Roh, H. Choi, J.-S. Kim, **H. Shin**, T. Park, K. Yong*, Low Power Consumed PV-Electrolysis with CoFeP Nanowires for Hydrazine-Assisted Hydrogen Production. *Appl. Surf. Sci.* **606**, 154951 (2022)
16. D. N. Nguyen, T. K. C. Phu, J. Kim, W. T. Hong, J.-S. Kim, S. H. Roh, H. S. Park, C.-H. Chung, W.-S. Choe, **H. Shin***, J. Y. Lee,* J. K. Kim*, Interfacial Strain-modulated Nanospherical Ni_2P by Heteronuclei-mediated Growth on Ti_3C_4TX MXene for Efficient Hydrogen Evolution. *Small* 2204797 (2022) **-highlighted as a front cover**
17. Y. Sun+, **H. Shin+**, F. Wang, B. Tian, C.-W. Chiang, S. Liu, X. Li, Y. Wang, L. Tang, W. A. Goddard*, M. Ding*, Highly Selective Electrocatalytic Oxidation of Amines to Nitriles Assisted by Water Oxidation on Metal Doped α-$Ni(OH)_2$. *J. Am. Chem. Soc.* **144**, 15185 (2022) **(co-1st Author)**
18. J. Min+, S. Kim+, A. A. Jeffery, **H. Shin**, Y. S. Kang, Y. Kim, J. Jang, S. Lee, S.-H. Park, G.-G. Park, S. J. Yoo, S.-D. Yim*, N. Jung*, A paradigm shift in CO tolerant catalyst design for fuel cells via introducing defect-controlled carbon molecular sieve layers, *Materials Today Energy* **29**, 101124 (2022)
19. S. Garain, C. D. Van, S. Choi, T. N. Dang, J. W. Ager, K. T. Nam, **H. Shin***, M. H. Lee*, Hierarchical Thiospinel $NiCo_2S_4$/Polyaniline Hybrid Nanostructures as a Bifunctional

Electrocatalyst for Highly Efficient and Durable Overall Water Splitting. *Adv. Mat. Interfaces* **9**, 2200649 (2022)

20. H. Y. Yoo, M. S. Kim, **H. Shin***, J. Lim*, Peroxymonosulfate Activation by Black TiO_2 Nanotube Arrays under Solar Light: Switching the Activation Mechanism and Enhancing Catalytic Activity and Stability. *J. Hazard. Mater.* **433**, 128796 (2022)
21. H. C. Kwon, Y. Park, J. Y. Park, R. Ryoo, **H. Shin***, M. Choi*, Catalytic Interplay of Ga, Pt, and Ce on the Alumina Surface Enabling High Activity, Selectivity, and Stability in Propane Dehydrogenation. *ACS Catal.* **11**, 10767 (2021)
22. B. Tian+, **H. Shin+**, M. Fei, S. Liu, Z. Mu, C. Liu, Y. Pan, Y. Sun, W. A. Goddard*, M. Ding*, Double Exchange Induced in situ Conductivity in Nickel Based Oxyhydroxides: An Effective Descriptor for Electrocatalytic Oxygen Evolution. *Angew. Chem. Int. Ed.* **60**, 2 (2021) **-selected as a Hot Paper (co-1st Author)**
23. N. Kim, T.-H. Gu, D. Shin, X. Jin, **H. Shin**, M. G. Kim, H. Kim*, S.-J. Hwang*, A Lattice Engineering Way to Simultaneously Control the Defect/Stacking Structures of Layered Double Hydroxide Nanosheets for Optimizing Their Energy Functionalities. *ACS Nano* **15**, 8306 (2021)
24. J. Wang, S.-J. Kim, J. Liu, Y. Gao, S. Choi, J. Han, **H. Shin**, S. Jo, J. Kim, F. Ciucci, H. Kim, Q. Li, W. Yang, X. Long, S. Yang, S.-P. Cho, K. H. Chae, M. G. Kim, H. Kim*, J. Lim*, Redirecting Dynamic Surface Restructuring of a Layered Transition Metal Oxide Catalyst for Superior Water Oxidation. *Nat. Catal.* **4**, 212 (2021) **-highlighted as a front cover**
25. C. Liu, J. Qian, Y. Ye, H. Zhou, C.-J. Sun, C. Sheehan, Z. Zhang, G. Wan, Y.-S. Liu, J. Guo, S. Li, **H. Shin**, S. Hwang, T. B. Gunnoe, W. A. Goddard*, S. Zhang*, Oxygen evolution reaction over catalytic single-site Co in a well-defined brookite TiO_2 nanorod surface. *Nat. Catal*. **4**, 212 (2021)
26. I. Jang, K. Im, **H Shin**, K.-S. Lee, H. Kim, J. Kim, S. J. Yoo*, Electron-deficient titanium single-atom electrocatalyst for stable and efficient hydrogen production. *Nano Energy* **78**, 105151 (2020)
27. L.-A. Huang+, **H. Shin+**, W. A. Goddard*, J. Wang*, Photochemically deposited Ir-doped NiCo oxyhydroxide nanosheets provide highly efficient and stable electrocatalysts for the oxygen evolution reaction. *Nano Energy* **75**, 104885 (2020) **(co-1st Author)**
28. D. H. Won, **H. Shin**, M. W. Chung, H. Jung, K. H. Chae, H.-S. Oh, Y. J. Hwang*, B. K. Min*, Achieving tolerant CO_2 electro-reduction catalyst in real water matrix, *Appl. Catal. B* **258**, 117961 (2019)
29. **H. Shin,** H. Xiao, W. A. Goddard*, In silico discovery of new dopants for Fe-doped Ni oxyhydroxide ($Ni_{1-x}Fe_xOOH$) catalysts for oxygen evolution reaction, *J. Am. Chem. Soc.* **140**, 6745 (2018) **-selected as one of the most highly cited publications in JACS for the period 2018-2019**
30. H. Xiao, **H. Shin,** W. A. Goddard*, The synergy between Fe and Ni in the Optimal Performance of (Fe,Ni)OOH Catalysts for the Oxygen Evolution Reaction, *Proc. Natl. Acad. Sci.* **115**, 5872 (2018)
31. S.-W. Baek, S. -H. Lee, J. H. Song, C. Kim, Y. -S. Ha, **H. Shin**, H. Kim, S. Jeong, J. -Y. Lee*, A hydro/oxo-phobic top hole-selective layer for efficient and stable colloidal quantum dot solar cells, *Energ. Environ. Sci.* **11**, 2078 (2018)
32. J. Lim, **H. Shin**, M. Kim, H. Lee, K.-S. Lee, Y. Kwon, D. Song, S. Oh, H. Kim, E. Cho*, Ga-doped Pt-Ni Octahedral Nanoparticles as a Highly Active and Durable Electrocatalyst for Oxygen Reduction Reaction, *Nano Lett.* **18**, 2450 (2018)
33. X. Jin, J. Lim, Y. Ha, N. H. Kwon, **H. Shin**, I. Y. Kim, N. S. Lee, M. H. Kim, H. Kim*, S. J. Hwang*, A critical role of catalyst morphology in low temperature synthesis of carbon nanotube−transition metal oxide nanocomposite. *Nanoscale* **9**, 12416 (2017)
34. I. Choi[+], H. Y. Jeong[+], **H. Shin**, G. Kang, M. Byun, H. Kim, A. M. Chitu, J. S. Im, R. S. Ruoff, S.-Y. Choi, K. J. Lee*, Laser-induced phase separation of silicon carbide. *Nat. Commun.* **7**, 13562 (2016)

35. **H. Shin**, Y. Ha, H. Kim*, 2D Covalent Metals: A New Materials Domain of Electrochemical CO_2 Conversion with Broken Scaling Relationship. *J. Phys. Chem. Lett.* **7**, 4124 (2016)
36. P. P. Upare, J. W. Yoon, D. W. Hwang, U.-H. Lee, Y. K. Hwang, D.-Y. Hong, J. C. Kim, J. H. Lee, S. K. Kwak, **H. Shin**, H. Kim, J.-S. Chang*, Design of a heterogeneous catalytic process for the continuous and direct synthesis of lactide from lactic acid. *Green Chemistry* **18**, 5978 (2016)
37. D. H. Won, **H. Shin**, J. Koh, J. Chung, H. S. Lee, H. Kim*, and S. I. Woo*, Highly Efficient, Selective, and Stable CO_2 Electroreduction on Hexagonal Zn Catalyst. *Angew. Chem. Int. Edi.* **55**, 1 (2016)
38. **H. Shin**, M. Choi, H. Kim*, Mechanistic Model for Hydrogen Activation, Spillover, and Its Chemical Reaction in Zeolite-Encapsulated Pt Catalyst. *Phys. Chem. Chem. Phys.* **18**, 7035 (2016) **(highlighted as an inside front cover)**
39. N. Jung+, **H. Shin+**, M. Kim, I. Jang, H.-J. Kim, E. Cho, J. H. Jang, H. Kim*, S. J. Yoo*, Janus Pt surfaces derivatized with zwitterionic molecules for oxygen reduction reactions in alkaline and acid electrolytes. *Nano Energy* **17**, 152 (2015) **(co-1st Author)**
40. D. Y. Chung, Y.-H. Chung, S. Kim, J. W. Lim, K. J. Lee, N. Jung, **H. Shin**, O.-H. Kim, H. Kim, S. J. Yoo*, Y.-E. Sung*, Understanding Interface between Electrode and Electrolyte: Organic/Inorganic Hybrid Design for Fast Ion Conductivity. *J. Phys. Chem. C* **119**, 9169 (2015)
41. J. Im+, **H. Shin+**, H. Jang, H. Kim, M. Choi*, Maximizing the catalytic function of hydrogen spillover in Platinum-encapsulated aluminosilicates with controlled nanostructures. *Nat. Commun.* **5**, 3370 (2014) **(co-1st Author)**
42. H.-K. Lim+, **H. Shin+**, W. A. Goddard, Y. J. Hwang, B. K. Min, H. Kim*, Embedding Covalency into Metal Catalysts for Efficient Electrochemical Conversion of CO_2. *J. Am. Chem. Soc.* **136**, 11355 (2014) **(co-1st Author)**
43. **H. Shin**, S. Jung, S. Bae, W. Lee*, H. Kim*, Nitrite Reduction Mechanism on a Pd Surface. *Environ. Sci. & Technol.* **48**, 12768 (2014)
44. S. Yook+, **H. Shin+**, H. Kim*, M. Choi*, Selective Dissociation of Dihydrogen over Dioxygen on a Hindered Platinum Surface for the Direct Synthesis of Hydrogen Peroxide. *ChemCatChem* **6,** 2836 (2014) **(co-1st Author)**
45. C. H. Choi, H. C. Kwon, S. Yook, **H. Shin**, H. Kim, M. Choi*, Hydrogen Peroxide Synthesis via Enhanced Two–Electron Oxygen Reduction Pathway on Carbon–Coated Pt Surface. *J. Phys. Chem. C* **118**, 30063 (2014)
46. C. H. Choi$^+$, H.-K. Lim$^+$, M. W. Chung, J. C. Park, **H. Shin**, H. Kim*, S. I. Woo*, Long Range Electron Transfer over Graphene-based Catalyst for High Performing Oxygen Reduction Reactions: Importance of Size, N-doping, and Metallic Impurities. *J. Am. Chem. Soc.* **136**, 9070 (2014)
47. D.-H. Seo, **H. Shin**, K. Kang, H. Kim*, S. S. Han*, First-Principles Design of Hydrogen Dissociation Catalysts Based on Isoelectronic Metal Solid Solutions. *J. Phys. Chem. Lett.* **5**, 1819 (2014)
48. B. J. Yang, **H. Shin**, H. Kim, H. K. Lee*, Strain rate and adhesive energy dependent viscoplastic damage modeling for nanoparticulate composites: Molecular dynamics and micromechanical simulations. *Appl. Phys. Lett.* **104**, 101901 (2014)
49. B. J. Yang, **H. Shin**, H. K. Lee, H. Kim*, A combined molecular dynamics/micromechanics/finite element approach for multiscale constitutive modeling of nanocomposites with interface effects. *Appl. Phys. Lett.* **103**, 241903 (2013)

50. **H. Shin**, T. A. Pascal, W. A. Goddard*, H. Kim*, Scaled Effective Solvent Method for Predicting the Equilibrium Ensemble of Structures with Analysis of Thermodynamic Properties of Amorphous Polyethylene Glycol-Water Mixtures. *J. Phys. Chem. B.* **117**, 916 (2013)