Byungchan Han

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Education

- Ph.D., Department of Materials Science and Engineering, **MIT**, 2007
- M.S., Department of Nuclear Engineering, **Seoul National University**, 2000
- B.S., Department of Nuclear Engineering, **Seoul National University**, 1998

Carrier

- **Professor**, **Yonsei University**, 2019 - Present
- Associate Professor, Yonsei University, 2015 - 2018
- Editor of **Applied Surface Science**, 2019 - Present
- Associate Editor of **NPG Scientific Reports**, 2016 - Present
- Editorial Board of Energy Materials (specialty section of Frontiers in Materials), 2021-current
- Reviewer Board of Royal Society of Chemistry, 2018 - Present
- National Committee for Pyroprocessing Technology of Spent Nuclear Fuel, 2018-2019 (USA-Korea Joint Project)
- Organizing Committee of The Asian Workshop on “First-Principles Electronic Structure Calculations”, 2018
- Organizing Board of Korean Institute of Hazardous Materials, 2018
- Board of the Korean Institute of Surface Engineering, 2016-Present
- Assistant, Associate Professor, DGIST, 2011 - 2014
- Vice Director of DGIST-LBNL Joint Research Center, 2012 - 2014
- Assistant/Associate Professor, DGIST, 2011-2014
- Postdoctoral Fellow, **Stanford University** (Mechanical Eng.), 2009 - 2011
- Postdoctoral Research Associate, **MIT** (Materials Sci. & Eng.), 2007 - 2009

Award

- **Ministry of Environment** for Environmental Safety Research,, 2020
- **Ministry of Science** & **Technology** for Leading Research in Nanotechnology, 2018
- International Association of Advanced Materials (IAAM) Medal, 2016, 2018
- Excellent Research Awards from Yonsei University, 2017, 2018
- Korea National Research Foundation for an Radioactive Chemistry, 2016
- Korean Electrochemical Society Award for a Best Paper, 2012
- Ten Most Leading Young Scientists Award, 2012
- Editor's choice for best paper in the multi-journal compilation of the latest research on nano-scale systems, American Physical Society 2005, 2006
- National Scholarship for studying Abroad, Ministry of Education, 2000
- Full Scholarship for B.S. & M.S. Programs, 1991-2000
- Alumni Award from Seoul National University, 2000
- Graduate with honors from Seoul National University, 1998

Biography

Byungchan Han is a tenured full professor at Department of Chemical & Biomolecular Engineering of Yonsei University in Seoul, Korea. He earned his PhD degree in MIT at the Dept. of Materials Science and Engineering in 2007. Before join to MIT He obtained Bachelor and Master degrees at Seoul National University. After his Ph.D program he spent two more years in **MIT** and another two years in **Stanford University** as Postdoctoral Research Associate. His research interests are developing emerging energy materials for renewable energy devices using **knowledge-based AI computings**. He was awarded by **Korea Ministry of Science & Technology** and **Ministry of Environment** for the Excellent Research work on Nanotechnology. Currently, he is an editor of Applied Surface Science and the editorial board of NPG Scientific Reports.

Research Interest:

- **Knowledge-based AI Machine Learning, DFT calculations**
- Clean/Renewable Energy Materials: Li-ion batteries, Fuel Cells, Electro/Photo Catalysts for Water Split & Fuel Production
- Computational Radiochemistry (Pyroprocess, Molten Salt, Phase Equilibria of UO_{2+x})
- Reaction Mechanism Prediction for Hazardous/Toxic Chemical
- MOF for Gas Phase Capture

Publication (2018-Present)

53. Selective Removal of Radioactive Iodine Species Using Electrochemically Reusable Magnetic Adsorbents, **Nature**, Submitted.
52. Bioinspired Catalytic Mononuclear CuN4 Center for the Partial Oxidation of Methane to Methanol, **Journal of the American Chemical Society,** Under Review.
51. Thermodynamic Origin and Growth Dynamics of Colloidal Nanoparticle Formation, **Nature**, Submitted
50. Genetic Manipulation of M13 Bacteriophage for Enhancing the Efficiency of Virus-Inoculated Perovskite Solar Cells With a Certified Efficiency of 22.3%, **Advanced Energy Materials**, Minor Revision.
49. Design of a Unique Anion Framework in Halospinel for Outstanding Performance of all Solid-State Li-Ion Battery: First-Principles Approach, **Journal of Materials Chemistry A**, Under Review.
48. Interfacing or Doping Role of Ce in Highly Promoted Water Oxidation of NiFe-Layered Double Hydroxide, **Advanced Energy Materials (VIP Paper)**, Minor Revision
47. First-Principles Based **Machine-Learning Molecular Dynamics** for Crystalline Polymers With Van der Waals Interactions, **Journal of Physical Chemistry Letters, Accepted (Front Cover).**
46. Laser-Ablated Red Phosphorus on Carbon Nanotube Film for Accelerating Polysulfide Conversion Towards High-Performance and Flexible Lithium–Sulfur Batteries, **Small Methods**, **Accepted**.
45. First-Principles Data Integrated **Machine-Learning** Approach for High-Throughput Searching of Ternary Electrocatalyst Towards Oxygen Reduction Reaction", **Chem Catalysis** (Cell Press), **Accepted**
44. Fluorine-decorated graphene nanoribbons for an anti-corrosive PEMFC, Applied Materials & Interface, **Accepted (**https://doi.org/10.1021/acsami.1c04132)

43. Dramatic Catalytic Activation of Kinetically Inert Disilane Hydrolysis in Metallic Iron Particulate via Barrierless Chemical Dissociation: First-Principles Study, **Applied Surface Science**, 560,14998 (2021).

42. Two-Dimensional Palladium Diselenide for Oxygen Reduction Reaction, **Materials Chemistry Frontiers**, in Press (DOI: 10.1039/D0Qm01113d)

41. n-Type Thermoelectric Properties of a Hexagonal SiGe Polymorph Superior to a Cubic SiGe, **Journal of Alloys and Compounds**, 874, 160007 (2021)

40. Unraveling the Selective Etching Mechanism of Silicon Nitride Over Silicon Dioxide by Phosphoric Acid: First-Principles Study, **Applied Surface Science**, 551, 149376 (2021)

39. Pore Tuning of Metal–Organic-Framework Membrane Anchored on Graphene-Oxide Nanoribbon, **Advanced Functional Materials**, 2011146 (2021)

38. Optical Bioelectronic Nose of Outstanding Sensitivity and Selectivity Toward Volatile Organic Compounds, **Biosensors and Bioelectronics** ,177, 112979 (2021)

37. Dominant Effect of Anharmonicity on the Equation of State and Thermal Conductivity of MgO Under Extreme Conditions, **Physical Review B**, 102, 184309 (2020)

36. Catalytic Activity of Ni3Mo Surfaces for Hydrogen Evolution Reaction: a Density Functional Theory Approach, **Applied Surface Science** 537, 14789 (2021)

35. High Quantum Efficiency and Stability of Biohybrid Nanojunctions in Bacteriophage-Constructed Perovskite Quantum Dots, **Materials Today Nano**, 13, 100099 (2021)

34. Ni Nanoparticles on Active (001) Facet-Exposed Rutile TiO2 Nanopyramid Arrays for Efficient Hydrogen Evolution, **Applied Catalysis B: Environmental**, 282, 1195482 (2021)

33. A Metal-Induced Self-Assembly Template for Controlled Growth of ZIF-8 Nanorods, **Chemistry of Materials**, 2020, 32, 18, 7941–7950 (2020)

32. Pairing of Transition Metal Dichalcogenide and Doped Graphene for Catalytically Dual Acive Interfaces for Hydrogen Evolution Reaction, **ACS Sustainable Chemistry & Engineering**, 8, 29, 10852–10858 (2020): **Front Cover**

31. Defect Structure Evolution of Polyacrylo1Nitrile and Single Wall Carbon Nanotube Nanocomposites: a Molecular Dynamics Simulation Approach, **NPG Scientific Reports**, 10, 11816 (2020)

30. First-Principles Mechanism Study on Distinct Optoelectronic Properties of Cl-Doped 2D Hybrid Tin Iodide Perovskite, **Journal of Materials Chemistry C**, 8, 9540-9548 (2020) : **Back Outside Cover**

29. Unique Design of Superior Metal-Organic Framework for Removal of Toxic Chemicals in Humid Environment via Direct Functionalization of the Metal Nodes, **Journal of Hazardous Materials**, 398, 122857 (2020)

28. Critical Differences in 3D Atomic Structure of Individual Ligand-Protected Nanocrystals in Solution, **Science, 03, 60-67 (2020): Front Cover**

27. Copper Phosphosulfides as a Highly Active and Stable Photocatalyst for Hydrogen Evolution Reaction, **Applied Catalysis B: Environmental**, 273, 118927 (2020)

26. Ultrastable Molybdenum Disulfide-Based Electrocatalyst for Hydrogen Evolution in Acidic Media, **Journal of Power Sources**, 456, 227998 (2020)

25. First-Principles Design of Highly Functional Sulfide Electrolyte Li10-xSnP2S12-xClx for all Solid-State Li-Ion Battery Applications, **ACS Sustainable Chemistry & Engineering**, 8, 3321-3327 (2020)

24. Thermochemical Study for Remediation of Highly Concentrated Acid Spill: Computational Modeling and Experimental Validation, **Chemosphere**, 247, 126098 (2020)

23. Size-Extensive Molecular **Machine Learning** With Global Representations, **ChemSystemsChem**, 2, E1900052 (2020); With Prof. Reuther's Group (Max Planck Institute)

22. Desulfurization of Hexyl Sulfide and Hexanethiol Using Supercritical Water, **Journal of Supercritical Fluids**, 158, 104734 (2020)

21. First-Principles Computational Study of Ni/A-Al2O3 Hybrid Interface Reactions Under Extreme Thermodynamic Conditions, **Applied Surface Science**, 509, 114861 (2020)

20. Design of Highly Efficient Adsorbents for Removal of Gaseous Methyl Iodide Using Tertiary Amine-Impregnated Activated Carbon: Integrated Experimental and First-Principles Approach, **Chemical Engineering Journal**, 373, 1003-1011 (2019)

19. Integrated Study of Experiment and First-Principles Computation for the Characterization of a Corium Type ZrO8 Complex in a Zr-Doped Fluorite UO2, **International Journal of Energy Research**, 43, 3322-3329 (2019)

18. Design of Active Bifunctional Electrocatalysts Using Single Atom Doped Transition Metal Dichalcogenides, **Applied Surface Science**, 471, 545-551 (2019)

17. First-Principles Computational Approach for Innovative Design of Highly Functional Electrocatalysts in Fuel Cells, **Current Opinion in Electrochemistry**, 12, 225-232 (2018), **Review Article**

16. First-Principles Computational Design of Unknown Flat Arsenene Epitaxially Grown on Copper Substrate, **Applied Surface Science**, 467-468, 561-566 (2019)

15. Unexpectedly High Energy Density of a Li-Ion Battery by Oxygen Redox in LiNiO2 Cathode: First-Principles Study, **Electrochimica Acta**, 294, 166-172 (2019)

14. Elucidation of Hydrolysis Reaction Mechanism of Tungsten Hexafluoride (WF6) Using First-Principles Calculations, **Journal of Industrial and Engineering Chemistry**, 70, 99-102 (2019)

13. First-Principles Prediction of Universal Relation Between Exchange Current Density and Adsorption Energy of Rare-Earth Elements in a Molten Salt, **Journal of Industrial and Engineering Chemistry**, 70, 94-98 (2019)

12. Tuning the Catalytic Activity of Heterogeneous Two-Dimensional Transition Metal Dichalcogenide for Hydrogen Evolution, **Journal of Materials Chemistry A (Back Cover)**, 6, 20005 (2018)

11. Understanding of Metals Encapsulated in Carbon Layers and Their Electrocatalytic Applications, **Accounts of Materials & Surface Research**, 3, 145-157 (2018) **Review Article**

10. First-Principles Database Driven Computational Neural Network Approach to the Discovery of Active Ternary Nanocatalysts for Oxygen Reduction Reaction, **Physical Chemistry Chemical Physics**, 20, 24539 - 24544 (2018)

9. Electrocatalytic Activity of Electrochemically Dealloyed $PdCu_3$ Intermetallic Compound Towards Oxygen Reduction Reaction in Acidic Media, **Journal of Material Chemistry A**, 6, 14828-14837 (2018)

8. Bifunctionally Active and Durable Hierarchically Porous Transition Metal-Based Hybrid Electrocatalyst for Rechargeable Metal-Air Batteries, **Applied Catalysis B: Environmenta**l, 239, 677-687 (2018)

7. The Effect of Alloying of Transition Metals (M = Fe, Co, Ni) With Palladium Catalysts on the Ele 4Ctrocatalytic Activity for the Oxygen Reduction Reaction in Alkaline Media, **Electrochimica Acta** 283, 1045-1052 (2018)

6. Universal Scaling Relationship To Screen an Efficient Metallic Adsorbent for. Adsorptive Removal of Iodine Gas Under Humid Conditions: First-Principles Study, **Journal of the Physical Chemistry C**, 122(22), 11799-11806 (2018)

5. First-Principles Study on Thermodynamic Stability of Hybrid Interfacial Structure of. LiMn2O4 Cathode and Carbonate Electrolyte in Li-Ion Battery, **Physical Chemistry Chemical Physics**, 20, 11592-11597 (2018) (**Back Cover)**

4. First Principles Computational Studies of Spontaneous Reduction Reaction of Eu(III) in Eutectic LiCl-KCl Molten Salt, **International Journal of Energy Research** (**Front Cover)**, 42, 2757-2765 (2018),

3. High Activity Hydrogen Evolution Catalysis by Uniquely Designed Amorphous/Metal Interface of Core–Shell Phosphosulfide/N-Doped CNTs, **Advanced Energy Materials** (**Communication**), 8(13), 1702806 (2018)

2. First-Principles Computational Screening of Highly Active Pyrites Catalysts for Hydrogen Evolution Reaction Through a Universal Relation With a Thermodynamic Variable, **Journal of the Physical Chemistry C**, 122(4), 2107-2112 (2018)

1. First Principles Computational Study on Hydrolysis of Hazardous Chemicals Phosphorus Trichloride and Oxychloride (PCl3 and POCl3) Catalyzed by Molecular Water Clusters, **Journal of Hazardous Materials**, 341 (5), 457-463 (2018)