

# Geun Ho Gu

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## Research Experience

|   |                  |
|---|------------------|
| <b>Assistant Professor</b> Korea Institute of Energy Technology (KENTECH)                           | 2/2022 – Present |
| <b>Post-Doctoral Research</b> Dr. Yousung Jung Lab, KAIST   | 4/2018 – 1/2022  |
| <b>Doctoral Research</b> Dr. Dion Vlachos Lab, University of Delaware (UD)                          | 1/2013 – 3/2018  |
| <b>Undergraduate Research</b> Dr. Paul Kenis Lab, University of Illinois at Urbana-Champaign (UIUC) | 5/2011 – 5/2012  |

## Education

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| <b>University of Delaware</b> PhD in Chemical Engineering                                     | 8/2012 – 5/2018 |
| <b>University of Illinois at Urbana-Champaign</b> BS in Chemical Engineering, Magna Cum Laude | 8/2008 – 5/2012 |

## Honors and Awards

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| <b>Outstanding Research Award</b> Korea Institute of Science and Technology Information              | 2022 |
| <b>Sejong Science Fellowship</b> National Research Foundation of Korea                               | 2021 |
| <b>Best Oral Presentation Award</b> The 9th Graduate Students Symposium in the CBE Department, KAIST | 2019 |
| <b>Distinguished Honor Student</b> , UIUC  | 2012 |
| <b>CITGO Award</b> , UIUC  | 2011 |
| <b>Omega Chi Epsilon</b> Chemical Engineering Honor Society  | 2011 |
| <b>Phi Eta Sigma</b> National Freshmen Honor Society   | 2008 |
| <b>Dean's List</b> , UIUC  | 2008 |

## External Support

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|---|-------------------------|
| <b>NRF Development of Simultaneous CO<sub>2</sub> Capture and Conversion Technology for Low Temperature Methanol Synthesis Using Active Learning Method</b> PI: Ung Lee | ₩250M, 2022-2026        |
| <b>Integrated Graduate School for Fuel Cell Power Generation</b> PI: Jonghee Han  | Total ₩4.75B, 2022-2027 |
| <b>KISTI Supercomputer Allocation</b> PI: Geun Ho Gu  | 22M SU, 2022-2023       |
| <b>NRF Sejong Science Fellowship</b> PI: Geun Ho Gu   | ₩450M, 2021-2026        |
| <b>KISTI Supercomputer Allocation</b> PI: Geun Ho Gu  | 17M SU, 2021-2022       |

## Service and Committees

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| <b>Review Editor</b> <i>Frontiers in Catalysis</i> (Frontiers Media) | 2020 – present |
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## Courses

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| <b>EF1002</b> Fundamentals of Chemistry, KENTECH             | Spring 2022, Spring 2023 |
| <b>EF6310</b> Artificial Intelligence for Chemistry, KENTECH | Fall 2022                |

## Selected Publications

(† indicates equal contribution. \* indicates a corresponding author)

- [1] **Autobifunctional Mechanism of Jagged Pt Nanowires for Hydrogen Evolution Kinetics via End-to-End Simulation**  
G. H. Gu, J. Lim, C. Wan, T. Cheng, H. Pu, S. Kim, J. Noh, C. Choi, J. Kim, W. A. Goddard, III\*, X. Duan\*, Y. Jung\* *J. Am. Chem. Soc.* **2021**, *143*, 5355-5363. IF 16.383 [Selected cover of the issue]
- [2] **Structure-Based Synthesizability Prediction of Crystals Using Partially Supervised learning**  
J. Jang†, G. H. Gu†, J. Noh, J. Kim, Y. Jung\* *J. Am. Chem. Soc.* **2020**, *142*, 18836-18843. IF 16.383
- [3] **Automated Exploitation of the Big Configuration Space of Large Adsorbates on Transition Metals Reveals Chemistry Feasibility**  
G. H. Gu\*, M. Lee, Y. Jung\*, D. G. Vlachos\* *Nat. Commun.* **2022**, *13*, 2087. IF 17.694

- [4] **Perovskite Synthesizability using Graph Neural Networks**  
G. H. Gu†, J. Jang†, J. Noh†, A. Walsh, Y. Jung\* *npj Comput. Mater.* **2022**, *8*, 71. IF 12.256
- [5] **Progress of Theoretical and Machine Learning Methods for Heterogeneous Small Molecule Activation**  
G. H. Gu†, C. Choi†, Y. Lee, A. B. Situmorang, J. Noh, Y. Kim\*, Y. Jung\* *Adv. Mater.* **2020**, *32*, 1907865. IF 32.086  
(Invited review)
- [6] **Predicting Potentially Hazardous Chemical Reactions Using Explainable Neural Network**  
J. Kim†, G. H. Gu†, J. Noh†, S. Kim, S. Gim, J. Choi, Y. Jung\* *Chem. Sci.* **2021**, *12*, 11028-11037. IF 9.969

## Publications and Proceedings

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(† indicates equal contribution. \* indicates a corresponding author)

- [28] **Dual-atom-site Sn-Cu/C3N4 photocatalyst selectively produces formaldehyde from CO2 reduction**  
B. Kim, D. Kwon, J. Baeg, M. Austeria, G. H. Gu, J. Lee, J. Jeong, W. Kim\*, W. Choi\* *Adv. Funct. Mater.*, *accepted*. IF 19.924
- [27] **Element-wise Formulation of Inorganic Retrosynthesis**  
S. Kim, J. Noh, G. H. Gu, S. Chen, Y. Jung\* *NeurIPS 2022 Workshop AI4Mat.* **2022**.
- [26] **Activity Trends of Methane Oxidation Catalysts under Emission Conditions**  
G. J. Bang†, G. H. Gu†, J. Noh, Y. Jung\* *ACS Catal.* **2022**, *12*, 10255. IF 13.700
- [25] **Perovskite Synthesizability using Graph Neural Networks**  
G. H. Gu†, J. Jang†, J. Noh†, A. Walsh, Y. Jung\* *npj Comput. Mater.* **2022**, *8*, 71. IF 12.256
- [24] **Automated Exploitation of the Big Configuration Space of Large Adsorbates on Transition Metals Reveals Chemistry Feasibility**  
G. H. Gu\*, M. Lee, Y. Jung\*, D. G. Vlachos\* *Nat. Commun.* **2022**, *13*, 2087. IF 17.694
- [23] **Bimetallic Gold–Silver Nanostructures Drive Low Overpotentials for Electrochemical Carbon Dioxide Reduction**  
J. W. Park, W. Choi, J. Noh, W. Park, G. H. Gu, J. Park, Y. Jung\*, H. Song\* *ACS Appl. Mater. Interface* **2022**, *14*, 6604-6614. IF 10.383
- [22] **Uncertainty Quantification and Error Propagation in the Enthalpy and Entropy of Surface Reactions Arising from a Single DFT Functional**  
G. Wittreich, G. H. Gu, D. Robinson, M. Katsoulakis, D. G. Vlachos\* *J. Phys. Chem. C* **2021**, *125*, 18187. IF 4.177
- [21] **Predicting Potentially Hazardous Chemical Reactions Using Explainable Neural Network**  
J. Kim†, G. H. Gu†, J. Noh†, S. Kim, S. Gim, J. Choi, Y. Jung\* *Chem. Sci.* **2021**, *12*, 11028-11037. IF 9.969
- [20] **Understanding Potential-dependent Competition Between Electrocatalytic Dinitrogen and Proton Reduction Reactions**  
C. Choi, G. H. Gu, J. Noh, H. S. Park, Y. Jung\* *Nat. Commun.* **2021**, *12*, 4353. IF 17.694
- [19] **Autobifunctional Mechanism of Jagged Pt Nanowires for Hydrogen Evolution Kinetics via End-to-End Simulation**  
G. H. Gu, J. Lim, C. Wan, T. Cheng, H. Pu, S. Kim, J. Noh, C. Choi, J. Kim, W. A. Goddard III\*, X. Duan\*, Y. Jung\* *J. Am. Chem. Soc.* **2021**, *143*, 5355-5363. IF 16.383 [Selected cover of the issue]
- [18] **Highly Stable Two-Dimensional Bismuth Metal-organic Frameworks for Efficient Electrochemical Reduction of CO<sub>2</sub>**  
F. Li, G. H. Gu, C. Choi, P. Kolla\*, S. Hong, T. Wu, Y. Soo, J. Masa, S. Mukerjee, Y. Jung\*, J. Qui, Z. Sun\* *Appl. Catal. B.* **2020**, *277*, 119241. IF 24.319
- [17] **Structure-Based Synthesizability Prediction of Crystals Using Partially Supervised learning**  
J. Jang†, G. H. Gu†, J. Noh, J. Kim, Y. Jung\* *J. Am. Chem. Soc.* **2020**, *142*, 18836-18843. IF 16.383
- [16] **Generative Adversarial Networks for Crystal Structure Prediction**  
S. Kim†, J. Noh†, G. H. Gu, A. Aspuru-Guzik, Y. Jung\* *ACS Cent. Sci.* **2020**, *6*, 1412-1420. IF 18.728
- [15] **Machine-enabled Inverse Design of Inorganic Solid Materials: Promises and Challenges**  
J. Noh, G. H. Gu, S. Kim, Y. Jung\* *Chem. Sci.* **2020**, *11*, 4871-4881. IF 9.969

- [14] **Uncertainty-Quantified Hybrid Machine Learning/Density Functional Theory High Throughput Screening Method for Crystals**  
J. Noh, G. H. Gu, S. Kim, Y. Jung\* *J. Chem. Inf. Model.* **2020**, *60*, 1996-2003. IF 6.162
- [13] **Progress of Theoretical and Machine Learning Methods for Heterogeneous Small Molecule Activation**  
G. H. Gu†, C. Choi†, Y. Lee, A. B. Situmorang, J. Noh, Y. Kim\*, Y. Jung\* *Adv. Mater.* **2020**, *32*, 1907865. IF 32.086 (Invited review)
- [12] **Practical Deep-Learning Representation for Fast Heterogeneous Catalyst Screening**  
G. H. Gu†, J. Noh†, S. Kim, S. Back, Z. Ulissi, Y. Jung\* *J. Phys. Chem. Lett.* **2020**, *11*, 3185-3191. IF 6.888
- [11] **Reduced Graphene Oxides with Engineered Defects Enable Efficient Electrochemical Reduction of Dinitrogen to Ammonia in Wide pH Range**  
M. Zhang, C. Choi, R. Huo, G. H. Gu, S. Hong, C. Yan, A. W. Robertson, J. Qui, Y. Jung\*, Z. Sun\* *Nano Energy.* **2020**, *68*, 104323. IF 19.069
- [10] **Unveiling New Stable Manganese based Photoanode Materials via Theoretical High-throughput Screening and Experiments**  
J. Noh, S. Kim, G. H. Gu, A. Shinde, L. Zhou, J. M. Gregoire\*, Y. Jung\* *ChemComm.* **2019**, *55*, 13418-13421. IF 6.065
- [9] **Lattice Convolutional Neural Network Modeling of Adsorbate Coverage-Effects**  
J. Lym†, G. H. Gu†, Y. Jung\*, D. G. Vlachos\* *J. Phys. Chem. C* **2019**, *123*, 18591-18959. IF 4.177 [Selected cover of the issue]
- [8] **Machine Learning for Renewable Energy Materials**  
G. H. Gu, J. Noh, I. Kim, Y. Jung\* *J. Mater. Chem. A.* **2019**, *7*, 17096-17117. IF 14.511 (Invited review)
- [7] **Microkinetic Modeling of Aqueous Phase Biomass Conversion: Application to Ethylene Glycol Reforming**  
G. H. Gu, G. R. Wittreich, D. G. Vlachos\* *Chem. Eng. Sci.* **2019**, *197*, 415-418. IF 4.889
- [6] **Thermochemistry of Gas-phase and Surface Species via LASSO-assisted Subgraph Selection**  
G. H. Gu, P. Plechac, D. G. Vlachos\* *React. Chem. Eng.* **2018**, *3*, 454-466. IF 5.200 [Selected front cover of the issue]
- [5] **Group Additivity for Aqueous Phase Thermochemical Properties of Alcohols on Pt(111)**  
G. H. Gu, B. Schweitzer, C. Michel, S. N. Steinmann\*, P. Sautet\*, D. G. Vlachos\* *J. Phys. Chem. C.* **2017**, *121* (39), 21510-21519. IF 4.177
- [4] **Group Additivity for Thermochemical Property Estimation of Lignin Monomers on Pt(111)**  
G. H. Gu, D. G. Vlachos\* *J. Phys. Chem. C.* **2016**, *120* (34), 19234-19241. IF 4.177
- [3] **Mechanism of Dehydration of Phenols on Noble Metals via First-Principles Microkinetic Modeling**  
G. H. Gu, C. A. Mullen, A. A. Boateng, D. G. Vlachos\* *ACS Catal.* **2016**, *6*, 3047-3055. IF 13.700
- [2] **Guaiacol Hydrodeoxygenation Mechanism on Pt(111): Insights from Density Functional Theory and Linear Free Energy Relations**  
K. Lee, G. H. Gu, C. A. Mullen, A. A. Boateng, D. G. Vlachos\* *ChemSusChem* **2015**, *8*, 315-322. IF 9.140
- [1] **Tailoring Electrode Hydrophobicity to Improve Anode Performance in Alkaline Media**  
M. S. Naughton, G. H. Gu, A. A. Moradia, P. J. A. Kenis\* *J. Power Sources* **2013**, *242*, 581-588. IF 9.794

## Presentations and Posters

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- [30] **Korean Chemical Society 131<sup>th</sup> General Meeting** G. H. Gu, *Enabling complex catalytic system simulation with machine learning* Suwon, Republic of Korea, 4/2023. (Presentation) [Invited Seminar]
- [29] **2023 Spring Meeting of the Korean Electrochemical Society** G. H. Gu, *Simulating complex catalytic system with machine learning* Jeju, Republic of Korea, 4/2023. (Presentation) [Invited Seminar]
- [28] **AI technology for Materials Research Data Workshop, KRISS** G. H. Gu *Data-science Accelerated Catalysis and Materials Research* Daejeon, Republic of Korea 1/2023. (Presentation) [Invited Seminar]
- [27] **Chung-Ang University** G. H. Gu *Interfacing Data Science for Accelerated Materials Research* Seoul, Republic of Korea 11/2022. (Presentation) [Invited Seminar]
- [26] **UNIST** G. H. Gu *Accelerating Materials Discovery with Synthesizability Prediction* Ulsan, Republic of Korea 10/2022. (Remote presentation) [Invited Seminar]

- [25] **2022 KICHE Fall Meeting and International Symposium** G. H. Gu *Data-science Accelerated Catalysis and Materials Research* Busan, Republic of Korea 10/2022. (Presentation)
- [24] **Industrial Engineering and Artificial Intelligence** G. H. Gu *Interfacing Data Science for Accelerated Materials Science* Busan, Republic of Korea 8/2022. (Presentation) [Invited Seminar]
- [23] **Application of Data Science in Materials Design and Materials Processing** G. H. Gu *Interfacing Data Science for Accelerated Materials Research* Seoul University, Republic of Korea 8/2022. (Presentation) [Invited Seminar]
- [22] **Inha University** G. H. Gu *Interfacing Data Science and Materials Science* Incheon, Republic of Korea 7/2022. (Presentation) [Invited Seminar]
- [21] **NACS North American Meeting** G. H. Gu, G. J. Bang, Y. Jung *Trends in Methane Oxidation on Rutile Oxide under Emission Conditions* New York City, NY, U.S. 5/2022. (Poster)
- [20] **2022 Spring Meeting of the Korean Electrochemical Society** G. H. Gu, *Interfacing Data Science and Materials Science* Jeju, Republic of Korea, 4/2022. (Presentation)
- [19] **Catalysis Webinar** G. H. Gu *AI Enhanced Computational Catalysis Science* Online. 11/2021. (Presentation) [Invited Seminar]
- [18] **Korean Chemical Society 128<sup>th</sup> General Meeting** G. H. Gu, J. Jang, J. Noh, A. Walsh, Y. Jung *Domain-Transfer Exploration of Perovskite Synthesizability with Positive and Unlabeled Learning* 10/2021. (Poster)
- [17] **AIChE Virtual Annual Meeting** G. H. Gu, J. Lim, C. Wan, T. Cheng, H. Pu, S. Kim, J. Noh, C. Choi, J. Kim, W. A. Goddard, III, X. Duan, Y. Jung *In-Situ Simulation of Jagged Pt Nanowire for Hydrogen Evolution Reaction* Online. 11/2020. (Presentation)
- [16] **International Conference on Molecular Simulation** G. H. Gu, J. Lim, C. Wan, B. Peng, T. Cheng, J. Noh, S. Kim, J. Kim, X. Duan, W. A. Goddard, III, Y. Jung *Unraveling the HER Mechanism of the Jagged Pt Nanowire via Machine Learning and Kinetic Monte Carlo* Jeju, Republic of Korea, 12/2019. (Poster)
- [15] **University of Delaware** G. H. Gu *Data-driven Modeling and Design for Sustainable Hydrogen Production*, Newark, DE, U.S. 7/2019. (Presentation) [Invited Seminar]
- [14] **NACS North American Meeting** G. H. Gu, M. Lee, Y. Jung, D. G. Vlachos *Predicting Multi-Dentate Adsorbate Conformation on Metal Surfaces* Chicago, IL, U.S. 6/2019. (Presentation)
- [13] **The 9<sup>th</sup> Graduate Student Symposium** G. H. Gu, J. Lim, S. Kim, J. Noh, J. Kim, Y. Jung *Machine Learning Enables Complex Surface Simulation: HER on Pt Jagged Nanowire* Daejeon, Republic of Korea. 5/2019. (Presentation)
- [12] **2019 Molecular Simulation** G. H. Gu, J. Lym, Y. Jung, D. G. Vlachos *Lattice Convolutional Neural Network for Modelling Adsorbate Coverage Effects* Gangwon-do, Republic of Korea. 1/2019. (Presentation)
- [11] **NACS North American Meeting** G. H. Gu, B. Schweitzer, C. Michel, S. N. Steinmann, P. Sautet, D. G. Vlachos *Group Additivity for Solvation Free Energy Estimation of Aliphatic Oxygenates on Pt(111)* Denver, CO, U.S. 6/2017. (Presentation)
- [10] **KAIST** G. H. Gu, D. G. Vlachos *Theoretical Approach to Biomass Conversion in Heterogeneous Catalysis* Daejeon, Republic of Korea, 12/ 2016. (Presentation) [Invited Seminar]
- [9] **CCEI Symposium** G. H. Gu, D. G. Vlachos *Fast Thermochemistry and Kinetics Estimation for Intermediates in Hydrodeoxygenation Reaction Network of Lignin Monomers* Newark, DE, U.S. 4/2016. (Poster)
- [8] **2015 Winter Research Review** G. H. Gu, D. G. Vlachos *Fast Estimation Methods of Catalytic Cycles of Lignin Molecules* Newark, DE, U.S. 1/2016. (Presentation)
- [7] **AIChE Annual Meeting** G. H. Gu, D. G. Vlachos *Fast Estimation Methods of Catalytic Cycles of Lignin Molecules on Pt(111)* Salt Lake City, UT, U.S. 11/2015. (Presentation)
- [6] **NACS North American Meeting** G. H. Gu, K. Lee, D. G. Vlachos *Computational Study of Hydrodeoxygenation of Lignin Compounds on Pt(111)* Pittsburgh, PA, U.S. 6/2015. (Poster)
- [5] **AIChE Annual Meeting** G. H. Gu, D. G. Vlachos *Hydrodeoxygenation Mechanisms of p-cresol on Pt(111)* Atlantic City, GA, U.S. 11/2014. (Presentation)
- [4] **CCST Research Review** G. H. Gu, D. G. Vlachos *DFT and Microkinetic Modeling of p-cresol Hydrodeoxygenation on Pt(111)* Newark, DE, U.S. 10/2014. (Poster)
- [3] **USDA FarmBio3 Annual Meeting** G. H. Gu, K. Lee, D. G. Vlachos *Modeling of Bio-oil Upgrade* Villanova, PA, U.S. 7/2014. (Presentation)

[2] **CCEI Symposium** G. H. Gu, D. G. Vlachos *DFT and Microkinetic Modeling of p-cresol Hydrodeoxygenation on Pt(111)* Newark, DE, U.S. 4/2014. (Poster)

[1] **USDA FarmBio3 Annual Meeting** G. H. Gu, K. Lee, D. G. Vlachos *Modeling of Catalytic Hydrodeoxygenation of p-cresol on Pt(111)*, Villanova, PA, U.S. 8/2013. (Presentation)

## Patents

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[1] **KR 10-2022-0134516** Y. S. Jung, G. H. Gu, J. H. Noh, J. D. Jang. *Perovskite synthesizability using graph neural networks and positive unlabeled learning*, Republic of Korea 10/19/2022. (Application)