

Guoxiang (Emma) Hu

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EDUCATION

- 2018 **PhD in Chemistry**, Department of Chemistry, University of California, Riverside
- 2013 **B.S. in Chemistry**, Department of Chemistry, University of Science and Technology of China

RESEARCH AND PROFESSIONAL EXPERIENCE

- 2023-present **Assistant Professor**, School of Materials Science and Engineering
Georgia Institute of Technology
- 2020-2023 **Assistant Professor**, Department of Chemistry and Biochemistry
Queens College of the City University of New York
- 2020-2023 **Doctoral Faculty of Chemistry**, Graduate Center of the City University of New York
- 2018-2020 **Postdoctoral Research Associate**; Supervised by: Dr. P. Ganesh
Oak Ridge National Laboratory, Center for Nanophase Materials Sciences
- Materials discovery *via* computational high-throughput and machine learning approaches
 - Strongly correlated quantum materials and their interfaces using quantum Monte Carlo
- 2013-2018 **Graduate Research Assistant**; Supervised by: Prof. De-en Jiang
University of California, Riverside, Department of Chemistry
- Surface chemistry and catalysis from first-principles
 - Structure-property relationships in atomically precise metal clusters

PEER-REVIEWED PUBLICATIONS

(**Overview:** Science, Nature Energy, Nat. Commun., J. Am. Chem. Soc.×4, Phys. Rev. Lett., Nano Lett.×2, Acc. Chem. Res., ACS Catal.×2, ACS Cent. Sci., Chem. Mater., J. Mater. Chem. A×4, ACS Appl. Mater. Interfaces×6, Nanoscale×2, J. Phys. Chem. Lett.×3, 9 corresponding-author papers, Google citation: 1899 (last updated 7/2023), * denotes the corresponding author, # denotes equal first-author contribution.)

As Assistant Professor at CUNY:

44. Brea, C.; **Hu, G.*** “Mechanistic Insight into Dual-Metal-Site Catalysts for Oxygen Reduction Reaction”, **ACS Catal.**, 2023, 13, 4992–4999.
43. Barman, K.; Askarova, G.; Jia, R.; **Hu, G.***; Mirkin, M.* “Efficient Voltage-Driven Oxidation of Water and Alcohols by an Organic Molecular Catalyst Directly Attached to a Carbon Electrode”, **J. Am. Chem. Soc.**, 2023, 145, 5786–5794.

42. Li, K.; Ding, L.; Xie, Z.; Yang, G.; Yu, S.; Wang, W.; Cullen, D.A.*; Meyer III, H. M.; Hu, G.; Ganesh, P.; Watkins, T. R.; Zhang, F.* “Robust Copper-Based Nanosponge Architecture Decorated by Ruthenium with Enhanced Electrocatalytic Performance for Ambient Nitrogen Reduction to Ammonia”, **ACS Appl. Mater. Interfaces**, 2023, 15, 11703–11712.
41. Boebinger, M. G.*; Brea, C.; Ding, L.; Misra, S.; Olunloyo, O.; Yu, Y.; Xiao, K.; Lupini, A. R.; Ding, F.; **Hu, G.**; Ganesh, P.; Jesse, S.; Unocic, R. R.* “The Atomic Drill Bit: Precision Controlled Atomic Fabrication of 2D Materials”, **Adv. Mater.**, 2023, 35, 2210116.
40. Wang, C.*; Malinoski, A.; Yuan, J.; Brea, C.; **Hu, G.** “A Surface Engineering Approach for Promoting Dexter Energy Transfer from Lead Halide Perovskite Nanocrystals” **J. Phys. Chem. C**, 2023, 127, 1135.
39. Zhang, Q.#; **Hu, G.#**; Starchenko, V.#; Wan, G.; Dufresne, E. M.; Dong, Y.; Liu, H.; Zhou, H.; Jeen, H.; Krogel, J. T.; Reboredo, F. A.; Lee, H.; Sandy, A. R.; Almazan, I. C.; Ganesh, P.*; Fong, D. D.* “Phase Transition Dynamics in a Complex Oxide Heterostructure”, **Phys. Rev. Lett**, 2022, 129, 235701.
38. Brea, C.; **Hu, G.*** “Shifting and Breaking Scaling Relations at Transition Metal Telluride Edges for Selective Electrochemical CO₂ Reduction”, **J. Mater. Chem. A**, 2022, 10, 10162-10170.
37. Xie, H.; Xie, X.; **Hu, G.***; Prabhakaran, V.; Saha, S.; Gonzalez-Lopez, L.; Phakatkar, A.; Hong, M.; Wu, M.; Shahbazian-Yassar, R.*; Ramani, V.; Al-Sheikhly, M.; Jiang, D.E.; Shao, Y.*; Hu, L.* “Ta–TiO_x Nanoparticles as Radical Scavengers to Improve the Durability of Fe–N–C Oxygen Reduction Catalysts”, **Nature Energy**, 2022, 7, 281–289.
36. Bennett, C.*#; **Hu, G.*#**; Wang, G.; Heinonen, O.; Kent, P.; Krogel, J. T.*; Ganesh, P.* “Origin of Metal-Insulator Transitions in Correlated Perovskite Metals”, **Phys. Rev. Res.**, 2022, 4, L022005.
35. Mazza, A.*; Lu, Q.; **Hu, G.**; Li, H.; Ankner, J.; Browning, J.; Charlton, T.; Brahlek, M.; Ward, Z.; Lee, H.; Ganesh, P.; Eres, G.* “Reversible Phase Transformations in La_{0.7}Sr_{0.3}MnO₃ Epitaxial Thin Films Driven by Hydrogen Induced Deoxygenation Characterized by In Situ Neutron Reflectometry”, **ACS Appl. Mater. Interfaces**, 2022, 14, 10898–10906.
34. Staros, D.#; **Hu, G.#**; Tiihonen, J.; Nanguneri, R.; Krogel, J.; Bennett, C.; Heinonen, O.; Ganesh, P.*; Rubenstein, B.* “A Combined First Principles Study of the Structural, Magnetic, and Phonon Properties of Monolayer CrI₃” **J. Chem. Phys.**, 2022, 156, 014707.
33. Barman, K.; Wang, X.; Jia, R.; **Hu, G.***; Mirkin, M.* “Voltage-driven Molecular Catalysis of Electrochemical Reactions” **J. Am. Chem. Soc.**, 2021, 143, 17344–17347.
32. Fung, V.*; Zhang, J.*; **Hu, G.**; Ganesh, P.; Sumpter, B. “Inverse Design of Two-dimensional Materials with Invertible Neural Networks” **npj Comput. Mater.**, 2021, 7, 200.
31. Malinoski, A.; **Hu, G.**; Wang, C.* “Strong Bidentate Coordination for Surface Passivation and Ligand-Shell Engineering of Lead Halide Perovskite Nanocrystals in the Strongly Quantum-Confined Regime” **J. Phys. Chem. C**, 2021, 125, 24521–24530.
30. Yan, Y.; Liu, C.; Yang, Y.; **Hu, G.**; Tiwari, V.; Jiang, D.E.; Peng, W.; Jha, A.; Duan, H.; Tellkamp, F.; Ding, Y.; Dai, S.; Shi, W.; Yuan, S.; Miller, D.; Ma, W.*; Zhao, J. “Deprotonation of TiO₂ Electron

- Transport Layer for Efficient and Stable Perovskite Solar Cells” **ACS Appl. Mater. Interfaces**, 2021, 13, 33, 39371-39378.
29. **Hu, G.***; Fung, V.; Huang, J.; Ganesh, P.* “Work Function Engineering of 2D Materials: The Role of Polar Edge Reconstructions”, **J. Phys. Chem. Lett.**, 2021, 12, 2320-2326.
28. Fung, V.*; **Hu, G.**; Ganesh, P.; Sumpter, B. “Machine Learned Features from Density of States for Accurate Adsorption Energy Prediction” **Nat. Commun.**, 2021, 12, 88.

Prior to CUNY:

27. Lu, Q.#; Sohn, C.#; **Hu, G.#**; Kylänpää1, I.; Krogel, J.; Kent, P.; Heinonen, O.; Ganesh, P.; Lee, H.* “Metal-Insulator Transition Tuned by Oxygen Vacancy Migration across VO₂/TiO₂ interface” **Sci. Rep.**, 2020, 10, 18554.
26. Fung, V.#; **Hu, G.#**; Jiang, D.E.* “Descriptors for Hydrogen Evolution on Single Atom Catalysts in Nitrogen-doped Graphene”. **J. Phys. Chem. C**, 2020, 124, 19571-19578.
25. Fung, V.; **Hu, G.**; Jiang, D.* “Hydrogen in Nanocatalysis”, **J. Phys. Chem. Lett.**, 2020, 11, 7049-7057.
24. Feng, J.; Yang, F.; **Hu, G.**; Yang, F.; Ye, Z.; Chen, J.; Yin, Y.* “Dual Roles of Polymeric Capping Ligands in the Surface-Protected Etching of Colloidal Silica”, **ACS Appl. Mater. Interfaces**, 2020, 12, 38751–38756.
23. Chen, J.; Li, B.; **Hu, G.**; Yang, F.; Lei, S.; Liu, D.; Lyu, F.; Wang, M.; Ge, X.; Zhang, Q.*; Yin, Y.* “An Integrated Evaporator for Highly Efficient Solar-Driven Interfacial Steam Generation”, **Nano Lett.**, 2020, 20, 6051–6058.
22. **Hu, G.***; Fung, V.; Sang, X.; Unocic, R. R.; Ganesh, P.* “Predicting Synthesizable Multi-Functional Edge Reconstructions in Two-Dimensional Transition Metal Dichalcogenides”, **Npj Comput. Mater.**, 2020, 6, 44.
21. Yang, H.; Chen, X.; **Hu, G.**; Chen, W.; Bradley, S.; Wu, X.; Zhang, W.; Verma, G.; Nann, T.; Jiang, D.E.; Kruger, P.; Zhang, J.; Tian, H.; Waterhouse, G.*; Telfer, S.*; Ma, S.* “Highly Efficient Electrocatalytic Hydrogen Evolution Promoted by O–Mo–C Interfaces of Ultrafine β-Mo₂C Nanostructures”, **Chem. Sci.**, 2020, 11, 3523-3530.
20. Fung, V.*; **Hu, G.**; Sumpter, B. “Electronic Band Contraction Induced Low Temperature Methane Activation on Metal Alloys” **J. Mater. Chem. A**, 2020, 8, 6057-6066.
19. **Hu, G.***; Fung, V.; Sang, X.; Unocic, R. R.; Ganesh, P.* “Superior Electrocatalytic Hydrogen Evolution at Engineered Non-stoichiometric Two-dimensional Transition Metal Dichalcogenide Edges”, **J. Mater. Chem. A**, 2019, 7, 18357-18364.
18. Fung, V.; **Hu, G.**; Tao, F.; Jiang, D. E.* “Methane Chemisorption on Oxide-Supported Pt Single Atom”, **ChemPhysChem**, 2019, 20, 2217-2220.
17. Zhou, M.; Higaki, T.; **Hu, G.**; Sfeir, M. Y.; Chen, Y.; Jiang, D. E.*; Jin, R.* “Three-Orders-of-Magnitude Variation of Carrier Lifetimes with Crystal Phase of Gold Nanoclusters”, **Science**, 2019, 364, 279-282.

16. Choi, W.; **Hu, G.**; Kwak, K.; Kim, M.; Jiang, D. E.*; Choi, J.P.*; Lee, D.* “Effects of Metal-Doping on Hydrogen Evolution Reaction Catalyzed by MAu₂₄ and M₂Au₃₆ Nanoclusters (M = Pt, Pd)”, **ACS Appl. Mater. Interfaces**, 2018, 10, 44645-44653.
15. Tang, Q.; **Hu, G.**; Fung, V.; Jiang, D. E.* “Insights into Interfaces, Stability, Electronic Properties, and Catalytic Activities of Atomically Precise Metal Nanoclusters from First Principles”, **Acc. Chem. Res.**, 2018, 51, 2793–2802.
14. **Hu, G.**; Wu, Z.; Jiang, D. E.* "First Principles Insight into H₂ Activation and Hydride Species on TiO₂ Surfaces", **J. Phys. Chem. C**, 2018, 122, 20323–20328.
13. Nair, L. V.; Hossain, S.; Takagi, S.; Imai, Y.; **Hu, G.**; Wakayama, S.; Kumar, B.; Kurashige, W.; Jiang, D. E.*; Negishi, Y.* “Hetero-Biicosahedral [Au₂₄Pd(PPh₃)₁₀(SC₂H₄Ph)₅Cl₂]⁺ Nanocluster: Selective Synthesis and Optical and Electrochemical Properties”, **Nanoscale**, 2018, 10, 18969-18979.
12. Hossain, S.; Ono, T.; Yoshioka, M; **Hu, G.**; Hosoi, M.; Chen, Z.; Nair, L.; Kurashige, W.; Jiang, D.E.*; Negishi, Y.* “Thiolate-Protected Trimetallic Au₂₀Ag₄Pd and Au₂₀Ag₄Pt Alloy Clusters with Controlled Chemical Composition and Metal Positions”, **J. Phys. Chem. Lett.**, 2018, 9, 2590-2594.
11. Li, W.; He, D.; **Hu, G.**; Li, X.; Banerjee, G.; Li, J.; Lee, S.; Dong, Q.; Brudvig, G.; Waagele, M.; Jiang, D.; Wang, D.* “Selective CO Production by Photoelectrochemical Methane Oxidation on TiO₂”, **ACS Cent. Sci.**, 2018, 4, 631-637.
10. **Hu, G.**; Wu, Z.; Jiang, D.E.* “Stronger-Than-Pt Hydrogen Adsorption in a Au₂₂ Nanocluster for Hydrogen Evolution Reaction”, **J. Mater. Chem. A**, 2018, 6, 7532-7537.
9. Meisner, Q.; Accardo, J.; **Hu, G.**; Clark, R.; Jiang, D.E.*; Zhu, L.* “Fluorescence of Hydroxyphenyl-Substituted "Click" Triazoles”, **J. Phys. Chem. A**, 2018, 122, 2956-2973.
8. **Hu, G.**; Wu, Z.; Dai, S.; Jiang, D.E.* “Interface Engineering of Earth-Abundant Transition Metals by Boron Nitride for Selective Electroreduction of CO₂”, **ACS Appl. Mater. Interfaces**, 2018, 10, 6694-6700.
7. You, B.[#]; Liu, X.[#]; **Hu, G.**[#]; Gul, S.; Yano, J.; Jiang, D.E.*; Sun, Y.* “Universal Surface Engineering of Transition Metals for Superior Electrocatalytic Hydrogen Evolution in Neutral Water”, **J. Am. Chem. Soc.**, 2017, 139, 12283-12290.
6. Foo, G.; **Hu, G.**; Hood, Z.; Li, M.; Jiang, D.; Wu, Z.*, “Kinetics and Mechanism of Methanol Conversion over Anatase Titania Nanoshapes”, **ACS Catal.**, 2017, 7, 5345-5356.
5. Wan, X.; Cheng, X.; Tang, Q.; Han, Y.; **Hu, G.**; Jiang, D.E.*; Wang, Q.* “Atomically Precise Bimetallic Au₁₉Cu₃₀ Nanocluster with an Icosidodecahedral Cu₃₀ Shell and an Alkynyl–Cu Interface”, **J. Am. Chem. Soc.**, 2017, 139, 9451-9454.
4. **Hu, G.**; Tang, Q.; Lee, D.; Wu, Z.; Jiang, D.E.* “Metallic Hydrogen in Atomically Precise Gold Nanoclusters”, **Chem. Mater.**, 2017, 29, 4840-4847. (Included in virtual issue *Chemistry of Materials for Water Splitting Reactions*: <https://pubs.acs.org/page/cmater/vi/water-splitting?ref=highlight>.)
3. **Hu, G.**; Jin, R.; Jiang, D.E.* “Beyond the Staple Motif: New Order at the Thiolate-gold Interface”, **Nanoscale**, 2016, 8, 20103-20110.

2. Wu, Z.*; **Hu, G.**; Jiang, D.; Mullins, D.; Zhang, Q.; Allard, L.; Wang, L.; Overbury, S. “Diphosphine-Protected Au₂₂ Nanoclusters on Oxide Supports Are Active for Gas Phase Catalysis Without Ligand Removal”, **Nano Lett.**, 2016, 16, 6560-6567.
1. **Hu, G.**; Tang, Q.; Jiang, D.E.* “CoP for Hydrogen Evolution: Implications from Hydrogen Adsorption” **Phys. Chem. Chem. Phys.**, 2016, 18, 23864-23871.

AWARDS/HONORS

2023	William Stewart Travel Award - CUNY Graduate Center
2023	NERSC DOE Mission Science Allocation Award, Award # BES-ERCAP0023976
2023	ORNL CNMS User Proposal, Award # CNMS2023-A-01910
2022	NERSC DOE Mission Science Allocation Award, Award # BES-ERCAP0020915
2022	PSC-CUNY Grant, “Boosting Hydrogen Production on Transition-Metal Dichalcogenides by Topological Surface States”, Award # 65381-00 53
2021	NERSC DOE Mission Science Allocation Award, Award # BES-ERCAP 0019036
2021	PSC-CUNY Grant, “Edge Engineering of Two-Dimensional Materials by Using Multiscale Simulations”, Award # 64396-00 52
2020	ORNL CNMS User Proposal, Award # CNMS2021-A-00595
2018	Award for Outstanding Self-Financed Students Abroad (China Scholarship Council)
2015	19 th International Society of Magnetic Resonance Conference Student Travel Award
2013	UCR Dean's Distinguished Fellowship
2010-2012	USTC Outstanding Student Scholarship
2009	USTC Outstanding Freshman Scholarship

TEACHING/SERVICE

Service:

2022-present	Reviewer for NSF and ACS PRF proposals.
2018-present	Reviewer for manuscripts in journals such as Nat. Energy, Nat. Commun., J. Phys. Chem. Lett., Carbon, J. Phys. Chem. C, ChemCatChem, ChemElectronChem, Int. J. Hydrogen Energy, etc.
2022-present	Alternate Delegate Senator on the Academic Senate.
2022	Judge in the WAC Lighting Foundation Invitational Science Fair
2022	Member of the Honors and Scholarships Committee at Queens College
2020-2021	Member of Strategic Plan Faculty Scholarship and Creativity Working Group at Queens College
2019	Basic Energy Sciences (BES) Early Career Network (ECN) Representative
2016	Materials Research Society Symposium Assistant, Boston, MA

Teaching:

Queens College, CUNY as Instructor:

Spring 2023 CHEM 1134 (General Chemistry I Lecture)
Spring 2022 CHEM 1134 (General Chemistry I Lecture)
Fall 2021 CHEM 3313/710 (Inorganic Chemistry/Advanced Inorganic Chemistry)
Spring 2021 CHEM 1134 (General Chemistry I Lecture)
Fall 2020 CHEM 3313/710 (Inorganic Chemistry/Advanced Inorganic Chemistry)

University of California, Riverside as Graduate Teaching Assistant:

2015-2017 CHEM 001-A/B/C (General Chemistry Lecture)
2013-2015 CHEM 001-LA/LB/LC (General Chemistry Laboratory)

Mentorship:

Graduate students: Courtney Brea, Hua Deng

Undergraduate students: Leeor Goldshmid, Daniel Yusupov, Aaron Goldblatt, Jordan Simkovic, Meir Breier,
Joshua Singavarapu

High school students: Deandrea Drackett, Anthony Palta

SELECTED PRESENTATIONS

June 2023 The 28th NAM of the North American Catalysis Society, Session co-chair, Providence, RI
Mar 2023 ACS Spring 2023 National Meeting, Invited Talk, Indianapolis, IN
Mar 2023 APS March Meeting 2023, Oral Presentation, Las Vegas, NV
Nov 2022 2022 Materials Research Society Fall Meeting, Oral Presentation, Boston, MA
Sep 2022 COPE 2nd Materials for Energy Harvesting and Conversion Workshop, Invited Talk, Atlanta, GA
Oct 2021 Chemistry Department Seminar, Invited Talk, College of Staten Island, CUNY, online
Mar 2021 MSE Department Seminar, Invited Talk, University of Texas at Arlington, online
Feb 2021 NYACS Computers in Chemistry Topical Group - Spring 2021 Seminar Series, Invited Talk
Dec 2020 GC Chemistry Seminar Day - Fall 2020, Invited Talk, CUNY, online
July 2020 Virtual Conference on Theoretical Chemistry 2020 (VCTC 2020), Poster Presentation, online
Mar 2020 ACS Spring 2020 National Meeting, Oral Presentation, online
Mar 2020 APS March Meeting 2020, Oral Presentation, online
Mar 2020 Chemistry Department Seminar, Invited Talk, Queens College, online
Feb 2020 Gordon Research Conference, Poster Presentation, Galveston, TX
Jan 2020 Chemistry Department Seminar, Invited Talk, Boston College, Boston, MA
Sep 2019 Southeastern Catalysis Society 18th Annual Fall Symposium, Oral Presentation, Knoxville, TN
Mar 2019 APS March Meeting 2019, Oral Presentation, Boston, MA
Jan 2019 Electronic Materials and Applications 2019, Oral Presentation, Orlando, FL

Nov 2018 2018 Materials Research Society Fall Meeting, Oral Presentation, Boston, MA
Mar 2018 ACS Spring 2018 National Meeting, Oral Presentation, New Orleans, LA
July 2017 6th International School for Materials for Energy and Sustainability, Poster Presentation, CA
Nov 2016 2016 Materials Research Society Fall Meeting, Oral Presentation, Boston, MA