Address: Department of Chemistry
University of Texas at Austin
1 University Station, A5300
Austin, TX, 78712-0165

Email: henkelman@utexas.edu
URL: http://henkelmanlab.org/
Tel: 512-769-3180

Date: December 2023

Birth: December 10, 1974
Vancouver, BC, Canada

RESEARCH INTERESTS

Atomistic simulations to determine materials properties of nanoscale systems.

Development of theory and computational methodology to extend the possible length and time scale of atomistic simulations.

Calculations based on density functional theory to describe atomic interactions such as chemical reactions at catalytic surfaces and the function of battery materials.

Computational design of materials for energy applications.

EDUCATION

1992-1996 Queen's University: Honors B.S. in Physics

1997-2001 University of Washington: Ph.D. in Theoretical Chemistry
Thesis Topic: Methods for Calculating Rates of Transitions with Application to Catalysis and Crystal Growth. Thesis Advisor: Dr. Hannes Jónsson

PROFESSIONAL APPOINTMENTS

2021-2022 Associate Chair, Department of Chemistry, University of Texas at Austin

2019-present George W. Watt Centennial Professor, Department of Chemistry, University of Texas at Austin

2015-2019 Professor, Department of Chemistry, University of Texas at Austin

2014-present Director, Center for Computational Molecular Sciences, Oden Institute for Computational and Engineering Sciences, University of Texas at Austin

2015-2016 Associate Chair of Chemistry, University of Texas at Austin

2010-2015 Associate Professor, Department of Chemistry, University of Texas at Austin

2004-2010 Assistant Professor, Department of Chemistry, University of Texas at Austin

2002-2004 Post-doctoral Researcher, Los Alamos National Laboratory

2001-2002 Post-doctoral Researcher, University of Washington

1997-2001 Graduate Student Research Assistant, University of Washington

SCHOLARSHIPS, AWARDS, and DISTINCTIONS

2023 Institute for Computational and Engineering Science Grand Challenge Faculty Award

2019 George W. Watt Centennial Professorship
2017 Peter O'Donnell Distinguished Research Award
2017 Institute for Computational and Engineering Science Grand Challenge Faculty Award
2013 Director, Center for Computational Molecular Sciences
2013 Faculty Research Assignment Award
2010 Institute for Computational and Engineering Science Grand Challenge Faculty Award
2007 National Science Foundation, CAREER Award
2002 Director's Postdoctoral Fellowship, Los Alamos National Laboratory
2000 IBM Graduate Student Award in Computational Chemistry
1998 Outstanding Student Service Prize
1998 The Ritter Fellowship
1993 The Arthur Louden Scholarship in Physics
1993 Hewlett Packard Award -- Top five students in Arts and Science

RECENT COLLABORATORS

Richard Crooks, John Goodenough, Adam Heller, Simon Humphrey, C. Buddie Mullins, Michael Rose, Charles Werth, Guihua Yu, and Jianshi Zhou (University of Texas at Austin), Anatoly Frenkel (Yeshiva), Judith Yang (University of Pittsburgh), Hannes Jónsson (University of Iceland), Arthur Voter (Los Alamos National Laboratory), Keith Stevenson (Skoltech), Sara Skrabalak (Indiana University), Yuan Chen (University of Sydney), Hyuck Mo Lee and Il-Doo Kim (KAIST), Tianyi Ma (University of Newcastle), Jinlong Gong (Tianjin University), Clare Grey (University of Cambridge), Maowen Xu (Chongqing University), Charles Sykes (Tufts University), Xiao Cheng Zeng (University of Nebraska-Lincoln), Guozhong Cao (Harbin Institute of Technology)

SYNERGISTIC ACTIVITIES

Reviewer: Regularly review articles for *J. Chem. Phys.*, *J. Phys. Chem.*, *Phys. Rev. B*, and *Lett.*, *Surf. Sci.*, *Nano. Lett.*, and proposals for the NSF and DOE.

Organizer: Symposium for the ACS Fall 2006 National Meeting
DOE-EFRC workshop in 2010
Telluride workshop on "Reaction Coordinates", Summer 2008
Telluride workshop on "Reaction Coordinates", Summer 2010
Telluride workshop on "Reaction Coordinates", Summer 2013
A three month (long) program "Materials for a Sustainable Energy Future" at IPAM, UCLA, Fall 2013
Telluride workshop on "Battery Workshop", Summer 2014
Telluride workshop on "Interfacial Chemistry and Charge Transfer for Energy Storage and Conversion", Summer 2016
A three month (long) program "Energy Landscapes", IPAM, UCLA, Fall 2017
Telluride workshop on "Computational Materials Chemistry", Summer 2014
MRS symposium "Advanced Atomistic Algorithms in Materials Science", 2017

Software: Maintain codes related to finding transition states, calculating reaction rates, and analysis of charge distribution from density functional theory. A website for these codes can be found at http://henkelmanlab.org/code/ and a discussion forum at http://henkelmanlab.org/forum/

Education: Leading a Freshman Research stream for the design of nanoparticle catalysts.

EDITORIAL and ADVISORY BOARDS

2021-present	Scientific advisory board: *Polaris Lithium*
2021-present	Editorial board: *Journal of Physical Chemistry*
2020-present	Editor: *Transactions of Tianjin University*
2020-present	Scientific advisory board: *Lantha Sensors*
2017	*Ad Hoc* Committee for Academic and Research Opportunities in Materials Science and Engineering
2014-2016	Steering committee: Texas Materials Institute
2012-2016	Science advisory board: Energy Frontier Research Center "Center for Atomic-level Catalyst Design"
2012-present	Editorial board: *Surface Science*
2012	Workshop advisory panel: Environmental Molecular Sciences Laboratory

RESEARCH GROUP

Postdoctoral Fellows:

Graduate Students: Jiyoung Lee, Mai Nguyen, Sai Pavan Jagannath Mantha, Naman Katyal, Benjamin Patterson, Eboni Williams, Ilgar Baghishov, Jaeyoung Cho, Jiaao Wang, Jiefeng Diao, Zahra Bajalan, and Sung Jung

Undergraduate Students:

Past Members (dates in group), current position and location:

Postdocs:
Hyunwoo Ha (2021-2023)
Kihyun Shin (2017-2022), Assistant Professor, Hanbat National University
Zhiyao Duan (2013-2021), Asst. Professor, Northwestern Polytechnical University
Wenrui Chai (2019-2020), Professor of Instruction, UT Austin
Lei Li (2016-2020), Associate Professor, SUSTech, Shenzhen, China
Ieuan Seymour (2020), Postdoc, Imperial College London
Hao Li (2019), Postdoc, Technical University of Denmark
Jin-Myoung Lim (2016-2017), Postdoc, University of Illinois
Penghao Xiao (2014-2016), Postdoc, Lawrence Livermore National Laboratory

Liang Zhang (2014-2015), Asst. Professor, Tsinghua University
Mrunalkumar Chaudhari (2013-2014), Lalbhai Dalpatbhai College of Engineering, India
Onise Sharia (2013-2014), Research Associate, Notre Dame
Alireza Ghasemi (2011-2013), Assistant Professor, IASBS, Iran
NaYoung Park (2011-2012) Postdoc, KAIST
HyunYou Kim (2010-2012) Assistant Professor, Chungnam National University, Korea
Gopi Krishna Phani Dathar (2009-2011) Applications Scientist, Schrödinger
Brad Dickson (2007-2009) Scientist, Van Andel Research Institute
Lijun Xu (2006-2008) Scientist, Honeywell UOP

PhD Students:
Ryan Ciufo (2015-2022), Postdoc, University of Texas at Austin
Hao Li (2015-2019), Postdoc, Technical University of Denmark
Wenrui Chai (2014-2018), Research Educator, University of Texas at Austin
Xinyu Li (2013-2018), Research Scientist, SES
Shannon Stauffer (2011-2016), Research Scientist, FTMC, Lithuania
Juliana Duncan (2010-2015), Research Educator, University of Texas
Liang Zhang (2009-2014), Asst. Professor, Tsinghua University
Samuel Chill (2009-2014), Software Engineer, Lantha Inc.
Penghao Xiao (2009-2014), Asst. Professor, Dalhousie University
Rye Terrell (2007-2013), Software Engineer at Zenoss
Zachary Pozun (2007-2012), Data Scientist, US Government
Nikolay Shestopalov (2008-2011), Technology Entrepreneur
Daniel Sheppard (2010), Staff Scientist, Los Alamos National Laboratory
Chun-Yaung Lu (2010), Scientist, Texas Advanced Computing Center
Wenjie Tang (2005-2010), Research Scientist, University of Minnesota

Masters Students:
Shen-Che Yang (2013-2015), PhD student, University of Texas

Undergraduate students (co-authors only):
Akksay Singh, (2019-2010) Graduate student, University of Texas at Austin
Benjamin Corona, (2013-2016) United States Army Institute of Surgical Research
Marco Howard, (2012-2014) Graduate student, University of Washington
Jeffrey Holzgrafe (2012) Undergraduate student, Olin College
Kelly Tran (2008-2011) Graduate student, Georgetown University
Matthew Welborn (2008-2011) Graduate student, MIT
Shingmei Chang (2008-2010) Graduate student, Navy dental school
Nathan Froemming (2007-2010) Graduate student, University of Washington
Travis Powell (2007-2009) Graduate student, University of Wisconsin

Visiting Scientists:
Seong Kyu Kim (2019-2020) Sungkyunkwan University, Korea
Meizan Jing (2019-) China University of Petroleum-Beijing, China
Huiling Zheng (2018-2019) China University of Petroleum-Beijing, China
Wanglai Cen (2017-2018) Sichuan University, China
Yulu Liu (2016-2018) Sichuan University, China

Anika Marusczyk (2015-2016) Bosch, Germany
Hui Fu (2011-2012) Qingdao, China
Hongxia Zhao (2011-2012) Shandong, China
Dahye Kim (2010) Korea Advanced Institute of Science and Technology
Jihoon Ryu (2009) Korea Advanced Institute of Science and Technology
Jakob Rasmussen (2009) Hammer group, Aarhus University

FUNDING AND SUPPORT

Lynas Rare Earths Inc.,
$50K (02/2022-01/2023)

Department of Energy, "Center for Materials for Water and Energy Systems (M-WET)" (PI Benny Freeman) $12M (08/2022-07/2026), DE-SC0019272.

National Science Foundation, "CCI Phase I: NSF Center for Single-Entity Nanochemistry and Nanocrystal Design" $1,800,000 (09/2022 – 88/2024), CHE- 2221062.

National Science Foundation, "CAS: Fundamental Experimental-Theoretical Investigations of New Metal Alloy Nanocatalysts for Natural Gas Repurposing" $589,346 (12/2021 – 12/2024), CHE-2109120.

National Science Foundation, "Computational methods for modeling reaction dynamics in batteries and catalysts" $450,000 (07/2021 – 07/2024), CHE-2102317.

Department of Energy, "Multimetallic Metal-Organic Frameworks as Heterogeneous Catalysts for Gas Phase Hydroformylation and Hydrogenation Reactions" (PI Donna Chen, University of South Carolina) $425,000 (09/2021-08/2024), DE-SC0019360.

National Science Foundation, "Computational methods for modeling reaction dynamics in batteries and catalysts" $450,000 (07/2021 – 07/2024), CHE-2102317.

Welch Foundation, "Design of materials for energy conversion and storage" $240,000 (06/2020 – 05/2023), F-1841.

Hyundai Motor Corporation, "Computational Study of Intermetallic Nanoparticles for Improved ORR Activity" $113,407 (09/2019 – 08/2020).

National Science Foundation, "Electrocatalytic Studies at Single, Structurally Well-defined Nanoparticles" (PI Richard Crooks) $495,000 (09/2019 – 08/2022), CHE-1855980.

National Science Foundation, "SusChEM: Non-precious metal substitution into hydrogenation metal alloy catalysts deposited onto redox active supports for facile nitrate destruction in drinking water" (PI Charles Werth),
$343,504 (09/2019 – 08/2022), CBET-1922504.

Department of Energy, "Testing the Predictive Power of Theory for Determining the Effect of Support Interactions on Electrocatalytic Nanoparticles" (PI Richard Crooks)
$650,000 (09/2019 – 09/2022), DE-SC0010576.

National Science Foundation, "Computational methodology to determine rare event chemical reaction dynamics and networks"
$469,470 (09/2018 – 08/2021), CHE-1764230.

National Science Foundation, "Bifunctional Catalysts for Selective Hydrogenation of Biomass Derivatives: Furfural Hydrogenation over Pt-Sn Supported on Titania" (PI Donna Chen)
$600,000 (09/2018 – 08/2021), CHE-1764164.

National Science Foundation, "Predictive Design and Scalable Synthesis of New Multimetallic Nanoparticles with Enhanced Surface Reactivity" (PI Simon Humphrey)
$435,000 (09/2018 – 08/2021), CHE-1807847

Office of Naval Research, "Automated characterization of chemical bonding in inorganic crystals" (PI Stefano Curtarolo)
$100,000 (09/2018 – 08/2019)

Sandia National Laboratory, "Implementation of Vineyard prefactor calculations for determining the rate of rare events using the Socorro density functional theory code"
$32,000 (06/2018 – 09/2018)

Welch Foundation, "Design of materials for energy conversion and storage"
$333,000 (06/2017 – 05/2020), F-1841.

ExxonMobil Research, "Extending atomic scale computational modeling of catalytic materials to human timescales"
$240,000 (06/2017 – 05/2019).

Department of Energy, "A Combined Experimental and Computational Approach to Understanding and Optimizing Nanoparticle/Support Interactions for Electrocatalysis" (PI Richard Crooks), DE-SC0010576
$650,000 (09/2016 – 09/2019).

National Science Foundation, "DMREF: Toolkit to Characterize and Design Bi-functional Nanoparticle Catalysts"
$1,240,000 (09/2015 – 08/2018), CHE-1534177

National Science Foundation, "Unconventional Noble Metal Nanoparticles with Enhanced Catalytic Properties: A Combined Experimental and Theoretical Study" (PI Simon Humphrey)
$483,000 (09/2015 – 08/2018), CHE-1505135

National Science Foundation, "CDS&E: Experimentally verified nano-oxidation simulations of Cu surfaces"
$315,000 (09/2014 – 08/2017), DMR-1410335.

Welch Foundation, "Design of materials for energy conversion and storage"
$180,000 (06/2014 – 05/2017), F-1841.

Department of Energy, "Testing the predictive power of theory for determining the structure and activity of nanoparticle electrocatalysts" (PI Richard Crooks)
$600,000 (09/2013 – 09/2016), DE-FG02-13ER16428.

Department of Energy, "SSAA: Ultra-high speed neutral plasma jets and their interactions with materials generating extreme conditions" (PI Mark Cappelli)
$801,000 (03/2013 – 02/2016), DE- FOA-0000611.

National Science Foundation, "Beyond harmonic transition state theory for accelerating molecular dynamics"
$492,000 (08/2012 – 07/2016), CHE-1152342.

Air Force Office of Scientific Research, "Fundamental study of interactions between pulsed high-density plasmas and materials for space propulsion" (PI Laxminarayan Raja)
$1,900,000 (07/2011 – 01/2016), FA9550-11-1-0062.

Department of Energy, "SISGR: Correlation of theory and function in well-defined bimetallic electrocatalysts" (PI Richard Crooks)
$912,000 (09/2009 – 08/2012), DE-FG02-09ER16090.

Department of Energy, "Energy frontier research center: Understanding charge separation and transfer at interfaces in energy materials and devices" (PI Paul Barbara, with 20 Co-PIs)
$16.5M (08/2009 – 07/2015), DE-SC0001091.

Texas Higher Education Board, Advanced Research Program, **"**Correlating the structure and function of bimetallic nanoparticles for catalysis" (with co-PI Prof. Richard Crooks)
$150,000 (05/2008 – 05/2010), 003658-0015-2007.

Welch Foundation, "First-principles calculations of catalytic reactions on metal surfaces and nanoparticles"
$150,000 (06/2008 – 05/2011), F-1601.

National Science Foundation, "CAREER: Methods for calculating molecular dynamics over long time scales"
$555,000 (03/2007 – 02/2012), CHE-0645497.

National Science Foundation, "NIRT: Functionalization of alloy metal nanoparticles for enhanced transport and catalysis in membranes" (PI Prof. B. Freeman)
$1,200,000 (10/2007 – 09/2011), CBET-0708779.

Texas Higher Education Board, Advanced Research Program, **"**Distributed computing environment for the rational design of catalysts from first principles" (co-PI Prof. V. Garg)
$65,000 (05/2006 – 05/2008), 003658-0022-2006.

Welch Foundation, **"**Modeling Nanoparticle Catalysts"
$150,000 (06/2005 – 05/2008), F-1601.

University of Texas at Austin, Summer Research Assignment: "Modeling nanoparticle catalysts"
$14,000 (06/2004 – 07/2004).

University of Texas at Austin, Startup Funds
$300,000 (09/2004 – 08/2008).

INVITED RESEARCH TALKS (total = 130)

12/2023 GetCO_2, Brisbane, AU
06/2023 GCIM2023, Jeju, Korea
01/2023 Alan Turing Institute, London
10/2021 Iowa State, Ames, IA
02/2020 ACS Student Chapter, UT
10/2019 AVS, Columbus, OH
08/2019 ACS, San Diego, CA
08/2019 Southern University, Shenzhen, China
07/2023 CECAM, Toulouse, France
02/2023 SIAM, Amsterdam
05/2022 University of Milano, Italy
06/2021 IPAM, Energy Landscapes, CA
02/2020 Washington State U., WA
09/2019 University of Buffalo, NY
08/2019 SINAP, Shanghai, China
08/2019 Sichuan University, Chengdu, China

08/2019 Beijing University of Chemical Tech**.**
04/2019 IMSE, WUSTL, St. Louis, MO
02/2019 CEC Meeting, Austin, TX
06/2018 CNLS, Santa Fe, NM
05/2018 Loughborough University (x2)
04/2018 University of South Carolina
10/2017 University of Wisconsin
08/2017 Telluride science research center
10/2016 IPAM, Collective Variables, UCLA
06/2016 IPAM MSEWR2, Arrowhead, CA
03/2016 ACS March Meeting, San Diego
01/2016 American Ceramic Society, Orlando
11/2015 MRS, Boston
10/2015 Condensed matter seminar, UT Austin
05/2015 ICCS workshop, Reykjavík, Iceland
04/2015 ACS, Denver
08/2014 FHI-AIMS developer, Berlin, UK
03/2014 APS, Denver
01/2014 Cornell University
10/2013 IPAM, MSEWS2, UCLA
09/2013 IPAM MSEWS tutorials, UCLA (x2)
07/2013 PsiK summer school, Norderney, DE
06/2013 Telluride science research center
11/2012 MRS, Boston
07/2012 ESF-LFUI, Energy landscapes, Austria
06/2012 Matgen IV, Santa Fe, NM
04/2012 Technical University of Denmark
03/2012 University of Pittsburgh
09/2011 UNM, Albuquerque
06/2011 Texas Advanced Computing Center
05/2011 EFRC summit, DC
03/2011 IPAM tutorial, UCLA
11/2010 Stanford, California
09/2010 PsiK 2010, Berlin, Germany
06/2010 Para2010, University of Iceland
04/2010 EFRC Thrust III Symposium, UT
11/2009 University of Montreal
10/2009 Nanoscience workshop, Grenoble
07/2009 ICAMS, Bochum, Germany
05/2009 DOE Contractor, Annapolis, VA
02/2009 Gordon Conference, Ventura, CA

05/2019 UC Riverside, Riverside, CA
03/2019 Oden Institute, Austin, TX
09/2018 University of Chicago, IL
05/2018 University Warwick
05/2018 University College London
02/2018 Mesilla electrochemistry workshop
09/2017 IPAM, CHDEL tutorials, UCLA (x2)
07/2017 DOE Contractors meeting, DC
07/2016 Telluride science research center
05/2016 North East Catalysis Society, Brown
01/2016 Mesilla Workshop, NM
01/2016 ExxonMobil Research, NJ
11/2015 CACDS seminar, U. Houston
07/2015 ICCB workshop, Kauai, Hawaii
04/2015 SurMat workshop, Düsseldorf
10/2014 Oklahoma University, OK
08/2014 Energy landscapes, Durham, UK
03/2014 ACS, Denver
12/2013 IPAM, MSE Culmination, Arrowhead
11/2013 IPAM, MSEWS4, UCLA
08/2013 University of Iceland, Reykjavik
06/2013 Telluride town talk
05/2013 ICAMS, Ruhr U., Bochum
11/2012 SWRM ACS, Baton Rouge
07/2012 CSTCC25, U. Guelph, Canada
06/2012 Telluride science research center
03/2012 MPI workshop, Dresden, Germany
11/2011 UT Dean's Scholars, Austin
07/2011 ACTC, Telluride, CO
06/2011 IPAM workshop, Lake Arrowhead
05/2011 IPAM workshop, UCLA
01/2011 Indiana University
10/2010 CalTech, California
09/2010 27th Max Born, Wroclaw, Poland
06/2010 Welch Summer Students, UT Austin
01/2010 University of Surrey, UK
10/2009 DOE workshop, Brookhaven
10/2009 Penn State University
06/2009 ACS Surface Science, New York
05/2009 IMA workshop, U. Minnesota
02/2009 IPAM workshop, UCLA

06/2008 IPAM reunion, Lake Arrowhead
04/2008 UT, Dallas
02/2008 Mesilla electrochemistry meeting
10/2007 ICES, Austin
10/2007 SMU, Dallas
08/2007 ACS, Boston
07/2007 IPAM reunion, Lake Arrowhead
05/2006 DOE, Washington, DC
09/2005 AMO seminar, UT Austin
05/2005 Surface Science Roundup, TX
03/2004 Denmark Technical University
05/2003 Minnesota: Electronic structure
12/2002 IAS, Princeton, NJ
06/2002 CECAM open source workshop, Lyon
04/2001 ACS, San Diego
06/2000 CECAM, Reykjavík, Iceland

01/2009 Wyatt symposium, UT Austin
10/2008 UW-Madison
06/2008 Telluride science research center
03/2008 YU, New York
08/2007 Texas advanced computing center
06/2007 Telluride science research center
09/2006 ACS, San Francisco
10/2005 IPAM, Los Angeles
07/2005 Dynamic Days, Berlin
03/2005 ACS, San Diego
03/2004 APS, Montreal
03/2003 ACS, New Orleans
11/2002 Ohio State University
04/2002 ICCN, Puerto Rico
05/2000 Sandia National Laboratory
06/1998 WCTC, PNNL

PUBLICATIONS (h-index = 82; citations > 70,000)

313. B. Kim, K. Shin, G. Henkelman and W.-H. Ryu, "CO_2-mediated Porphyrin Catalysis in Reversible Li-CO_2 Cells" *Chem. Eng. J.* **477**, 14741 (2023).

312. Y. Wang, N. Katyal, Y. Tang, H. Li, K. Shin, W. Liu, R. He, M. Xu, G. Henkelman and S.-J. Bao, "One-step pyrolysis construction of bimetallic atom-cluster sites for boosting bifunctional catalytic activity in Zn-air batteries" *Small* (in press, 2023).

311. Z. Wang, J. Diao, J. N. Burrow, K. K. Reimund, N. Katyal, G. Henkelman, and C. B. Mullins, "Urea-Modified Ternary Aqueous Electrolyte with Tuned Intermolecular Interactions and Confined Water Activity for High-Stability and High-Voltage Zinc-Ion Batteries" *Adv. Func. Mater* (in press, 2023).

310. H. Zhang, J. Diao, Y. Liu, H. Zhao, B. K. Y. Ng, Z. Ding, Z. Guo, H. Li, J. Jia, C. Yu, F. Xie, G. Henkelman, M.-M. Titirici, J. Robertson, P. Nellist, C. Duan, Y. Guo, D. J. Riley, and J. Qiu, "In-Situ Grown Cu Dendrites Plasmonically Enhance Electrocatalytic Hydrogen Evolution on Facet-Engineered Cu_2O" *Adv. Mater* **35**, 2305742 (2023).

309. X. Chi, M. Li, X. Chen, J. Xu, X. Yin, S. Li, Z. Jin, Z. Luo, X. Wang, D. Kong, M. Han, J.-J. Xu, Z. Liu, D. Mei, J. Wang, G. Henkelman, and J. Yu, "Enabling High-Performance All-Solid-State Batteries via Guest Wrench in Zeolite Strategy" *J. Am. Chem. Soc.* **145**, 24116-24125 (2023).

308. W. Guo, S. Wang, Y. Xie, C. Fang, L. Liu, Q. Lou, X. Lian, and G. Henkelman, "Hydrogen Peroxide Synthesis via Electrocatalytic Water Oxidation on sp^3 and sp^2 Carbon Materials Mediated by Carbonates and Bicarbonates" *ACS Sustain. Chem. Eng.* **11**, 12114-12122 (2023).

307. L. Li, R. A. Ciufo, J. Lee, C. Zhou, B. Lin, and G. Henkelman, "Atom-Centered Machine-Learning Force Field Package" *Comp. Phys. Comm.* **292**, 108883 (2023).

306. H. Ha, C. Lee, J. S. Park, C.-H. Chung, S. Lee, G. Henkelman, H. Y. Kim, and K. Shin, "Genetically Evolved Graphene Encapsulated Random Alloy Nanoparticles for Li-Air Battery" *Catal. Today* **424**, 114303 (2023).

305. P. Kunal, C. Yan, H. Guo, H. Li, C. Brady, M. Duncan, X. Zhan, C. Werth, G. Henkelman, and S. Humphrey, "Pd-Au-Cu Ternary Alloy Nanoparticles: Highly Tunable and Economical Nitrite Reduction Catalysts" *ACS Catal.* **13**, 11945-11953 (2023).

304. C. Du, S. Lu, J. Wang, X. Wang, M. Wang, H. Fruehwald, L. Wang, B. Zhang, T. Guo, J. Mills, W. Wei, Z. Chen, Y. Teng, J. Zhang, C. Sun, H. Zhou, R. Smith, B. Kendall, G. Henkelman, and Y. Wu, "Selectively reducing nitrate into NH_3 in neutral media by PdCu single-atom alloy electrocatalysis" *ACS Catal.* **13**, 10560-10569 (2023).

303. Y. Wang, H. Dong, N. Katyal, B. S. Vishnugopi, M. K. Singh, H. Hao, Y. Liu, P. Liu, P. P. Mukherjee, G. Henkelman, J. Watt, and D. Mitlin, "Intermetallics based on Sodium Chalcogens Promote Stable Electrodeposition – Electrodissolution of Sodium Metal Anodes" *Adv. Energy Mater.* **13**, 2204402 (2023).

302. P. Gao, Z. Liu, J. Diao, J. Wang, J. Li, Y. Tan, G. Hai, and G. Henkelman, "Calculated Outstanding Energy-storage Media by Aluminum-decorated Carbon Nitride (g-C_3N_4): Elucidating the Synergistic Effects of Electronic Structure Tuning and Localized Electron Redistribution" *Crystals* **13**, 655 (2023).

301. D. Guo, J. Wang, T. Lai, G. Henkelman, and A. Manthiram, "Electrolytes with Solvating Inner Sheath Engineering for Practical Na-S Batteries" *Adv. Mater.* **35**, 2300841 (2023).

300. C. Lee, K. Shin, Y. Park, Y. H. Yoon, G. Doo, G. H. Jung, M. Kim, W. C. Cho, C.-H. Kim, H. M. Lee, H. Y. Kim, S. Lee, G. Henkelman, and H.-S. Cho, "Catalyst–Support Interactions in Zr_2ON_2-supported IrO_x Electrocatalysts to Break the Trade-off Relationship between the Activity and Stability in the Acidic Oxygen Evolution Reaction" *Adv. Func. Mater.* **33**, 2301557 (2023).

299. S.-H. Kim, K. Shin, X. Zhou, C. Jung, H. Y. Kim, S. Pedrazzini, M. Conroy, G. Henkelman, and B. Gault, "Atom probe analysis of $BaTiO_3$ enabled by metallic shielding" *Scr. Mater.* **229**, 115370 (2023).

298. J. Eichler, J. Burrow, N. Katyal, G. Henkelman, and C. B. Mullins, "Modulation of CO_2 Adsorption Thermodynamics and Selectivity in Alkali-Carbonate Activated N-Rich Porous Carbons" *J. Mater. Chem. A* **11**, 12811-12826 (2023).

297. K. Liu, J. Wang, C. Lou, Z. Zhou, N. Zhang, Y. Yu, Q. Zhang, G. Henkelman, M. Tang, and J. Sun, "Simple Construction and Reversible Sequential Evolution Mechanism of Nitrogen-doped Mesoporous Carbon/SnS_2 Nanosheets in Lithium-ion Batteries" *Appl. Surf. Sci.* **618**, 156673 (2023).

296. H. Zhang, J. Diao, M. Ouyang, H. Yadegari, M. Mao, M. Wang, G. Henkelman, F. Xie, and D. J. Riley, "Heterostructured Core–Shell Ni–Co@ Fe–Co Nanoboxes of Prussian Blue

Analogues for Efficient Electrocatalytic Hydrogen Evolution from Alkaline Seawater" *ACS Catal.* **13**, 1349-1358 (2023).

295. P. Gao, Z. Liu, J. Zhang, J. Wang, and G. Henkelman, "A Fast, Low-cost and Simple Method for Predicting Atomic/Inter-atomic Properties by Combining a Low Dimensional Deep Learning Model with a Fragment based Graph Convolutional Network" *Crystals* **12**, 1740 (2022).

294. Y. Zhu, J. Wang, T. Koketsu, M. Kroschel, J.-M. Chen, S.-Y. Hsu, G. Henkelman, Z. Hu, P. Strasser, and J. Ma, "Iridium single atoms incorporated in Co_3O_4 efficiently catalyze the oxygen evolution in the acidic condition" *Nature Commun.* **13**, 7754 (2022).

293. Y. Wang, Y. Liu, M. Nguyen, J. Cho, N. Katyal, H. Hao, R. Fang, N. Wu, J. Nanda, G. Henkelman, J. Watt, and D. Mitlin, "Stable Anode-Free All-Solid-State Lithium Battery through Tuned Metal Wetting on the Copper Current Collector" *Adv. Mater.* **35**, 2206762 (2022).

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