

YANG SHAO-HORN

Massachusetts Institute of Technology

Professor Shao-Horn is the JR East Professor of Engineering and Professor of Materials Science and Engineering at Massachusetts Institute of Technology (M.I.T.). Professor Shao-Horn earned her B.S. degree from Beijing University of Technology and her Ph.D. degree from Michigan Technological University both in Metallurgical and Materials Engineering. She joined M.I.T. faculty in 2002.

Professor Shao-Horn's research is centered on exploiting physical chemistry principles to understand and design charge transfer and dynamics at interfaces, critical to enable clean energy for decarbonization and mitigate climate change. Professor Shao-Horn and coworkers have pioneered the use of electronic structure features to develop guiding principles of kinetics, ion mobility and dynamics to enhance functions across a number of applications spanning from making of sustainable fuels and chemicals from reduction of water, CO₂ or nitrogen, to rechargeable lithium-ion and lithium-air batteries. Research programs include experimental and computational components including synthesis, (electro)chemical measurements, synchrotron X-ray diffraction and spectroscopy, electron- and light-based imaging and spectroscopy, Density Functional Theory computation and machine learning. Professor Shao-Horn and her coworkers are highly interdisciplinary and collaborate closely with other leading labs and private sectors in chemical, automotive, and energy industries. Select research results from the past few years are described in detail below.

Professor Shao-Horn and her coworkers have tuned the oxide electronic structure to develop active and non-precious-metal-containing catalysts to promote oxygen reduction and evolution kinetics (accounting for ~75% of total energy loss), which is central to achieve high efficiencies of water-splitting devices, fuel cells, and metal-air batteries. The oxide electronic structure features, more specifically the energy levels of metal d and O p density of states (DOS), dictate the filling of antibonding orbitals on metal and oxygen sites, metal-oxygen covalency, and the binding strength with reaction intermediates, which influences the reaction energetic barrier for the rate-limiting step and thus reaction kinetics. Shao-Horn and her collaborators have also shown that the antibonding orbital filling ("e_g" 3d electron) of surface transition-metal cations controls the catalytic activity of oxides for oxygen reduction (Suntivich et al. Nature Chemistry 2011) and oxygen evolution (Suntivich et al. Science 2011) in a volcano-shaped dependence over several orders of magnitude. Applying this principle to design new oxide chemistry has led to intrinsic oxygen evolution activity greater than start-of-the-art IrO₂ (Suntivich et al. Science 2011) and record intrinsic oxygen reduction activity for non-precious-metal-based catalysts known to date (Stoerzinger et al. JPCL 2015). Shao-Horn and her coworkers have established criteria to obtain high stability and activity of most active catalysts for oxygen evolution, where increasing the metal-oxygen covalency (smaller energy gap between metal d and O 2p states) enhances activity but beyond an optimal value reduces oxide stability (May et al. JPCL 2012 and Grimaud et al. Nature Comm 2013). Exploiting this concept to examine a series of oxides not only sets record catalytic activity but also establishes a new reaction mechanism for the most active oxides, where both metal and oxygen sites can catalyze oxygen evolution (Grimaud et al. Nature Chemistry 2017) and deprotonation from oxide surface can be rate-limiting (Hong et al. EES 2017) – contrary to long-standing belief. Therefore, tuning metal-covalency and activating surface oxygen sites points to a new direction to increase oxide activity and stability. Recently, such concepts have been applied in the design of surfaces to suppress the dehydrogenation of electrolytes to enhance the lifetime and safety of high-energy Li-ion batteries (Giordano et al. JPCL 2017, Yu et al., JPCC 2018 and Zhang et al., EES 2020) and selective oxidation of hydrocarbon fuels (Advanced Energy Materials 2020).

Professor Shao-Horn and coworkers have made notable contributions to advance the development of fuel cells for consumer vehicles. Her work on the mechanism of Pt catalyst loss in fuel cells in collaboration with GM has contributed to prolonging the lifetime of fuel cells from hundreds to thousands of hours and to the first commercialization of fuel-cell-powered vehicle, Mirai, by Toyota in 2015. In addition, Shao-Horn and her coworkers have established the degradation mechanisms of Pt and Pt alloy nanoparticles in fuel cells (Ferreira et al. JES 2005 and Chen et al. JES 2010). Recent work has demonstrated record ORR activity for Pt alloy catalysts in fuel cells exceeding the target set by US Department of Energy for 2017 by teaming up with GM and Johnson Matthey (EES 2015).

Professor Shao-Horn and collaborators have shown that lattice dynamics can be used to control ion mobility in solid state electrolytes, where lowering the phonon DOS of mobile ions such as lithium and sodium reduces activation energy and promote ion mobility (Chem Review 2016, EES 2018 and JACS 2018). Such school of thoughts are being used to search and discover new solid state electrolytes (iScience 2019). Ongoing efforts are centered on developing a unified framework and descriptor on liquid, polymer and solid-state ceramic electrolytes (Qiao et al., ACS Central Science 2020).

Mostly recently, Professor Shao-Horn and collaborators have shown that tuning non-covalent interactions and solvation environments at the electrified interface can significantly the kinetic barriers for electron transfer and proton transfer and alter the rates of electron transfer (Huang et al, JPCC 2021) and proton-concerted electron transfer reactions including hydrogen evolution/oxidation (Huang et al. JACS Au 2021) and oxygen reduction (Tao et al., Nature Catalysis 2021). Such concepts are being used to control the selectivity of N₂ and CO₂ reduction to make fuels from electricity from Solar/Wind.

Professor Shao-Horn is a member of National Academy of Engineering, and is among the World's Most Influential Scientific Minds and *Highly Cited Researchers* (Thomson Reuters) based on ~390 archival journal papers (~64,700 citations and h-index of 120 on Google Scholar) and ~300 invited, keynote and plenary lectures in academia (e.g. Marvel Lecture 2017 and Cardona Lecture 2019), at industrial events (e.g., BASF Energy Symposium in 2015) and high-level strategic meetings (e.g., Ideaslab of World Economic Forum in Davos 2017). She has advised ~100 students and postdoctoral associates at MIT, who are now pursuing successful careers in industry, national research laboratories, and in academia (~35) including faculty positions at Northwestern, University of Michigan, MIT, and Cornell and academic positions in Europe and Asia.

Professor Shao-Horn's leadership and service contributions include: MIT *Climate Grand Challenges* program, MIT Energy Council, Co-Director for Center for Energy Storage at MIT; Energy Area Head of MIT Mechanical Engineering; National Science Foundation Interdisciplinary Leader. In addition, she has been serving on the Board of Directors including IMLB, advisory boards of private/public organizations including SLAC SUNCAT, PNNL, ENSUS research chair at Mohammed VI Polytechnic University, and the Fritz Haber Institute of Max Planck Society. Moreover, Professor Shao-Horn serves as Senior Editor for Accounts of Materials Research of American Chemical Society (ACS), and on advisory/editorial boards of leading journals including the Journal of Physical Chemistry and Materials Letters in ACS, Energy and Environmental Science from Royal Society of Chemistry (RSC), Advanced Energy Materials from Wiley and Cell Press Chem and Joule.

YANG SHAO-HORN

EDUCATION

Ph.D. in Metallurgical & Materials Engineering (May 1998)

Michigan Technological University, Houghton, MI 49931

Dissertation: The structural stability of transition metal oxides for lithium rechargeable cells.

Research Advisor: Professor Stephen A. Hackney

B.S. in Metallurgical & Materials Engineering (July 1992)

Beijing University of Technology, Beijing, P.R. China

EMPLOYMENT

JR East Professor of Engineering	7/2021-present
Professor of Mechanical Engineering and Materials Science and Engineering	7/2020-present
W.M. Keck Professor of Energy, MIT	7/2015-6/2020
Gail E. Kendall Chair in Mechanical Engineering, MIT	7/2011-6/2015
Associate Professor, Department of Mechanical Engineering, MIT	7/2007-6/2011
Assistant Professor, Department of Mechanical Engineering, MIT	8/2002-7/2007
Staff Materials Scientist, Eveready Battery Company, Cleveland	6/1998-10/2000

PROFESSIONAL SOCIETIES

Materials Research Society (1998-present)

American Chemical Society (2002-present)

HONORS and AWARDS

Highly Cited Research (2022); Falling Walls Finalist in Physical Sciences (2022); Hans Fischer Senior Fellow of the Technical University of Munich (2022); J.R. East Professor of Engineering (2021); Humboldt Research Prize in Chemistry (2020); Fellow of the National Academy of Inventors (2020); Dr. Karl Wamsler Innovation Award of the Technical University of Munich (2020); Highly Cited Researcher (2015-present); Mok Hing Yiu Distinguished Visiting Professorship at the Hong Kong University (2019); Faraday Medal from Royal Society of Chemistry (2018); Election to the National Academy of Engineering (2018); Fellow of the International Society of Electrochemistry (2018); Fellow of the Electrochemical Society (2017); Battery Research Award of the Electrochemistry Society (2016); Singapore Research Professorship (2015); Fellow of Royal Society of Chemistry (2014); Fellow of American Association for the Advancement of Science 2014; International Battery Association Research Award (2013); Charles W. Tobias Young Investigator Award of the Electrochemical Society (2008); Tajima Prize of the International Society of Electrochemistry (2008); Invited Professorship at the Université de Nantes (2008-2009), 3M Innovation Award Fund (2007), Battery Division Officer of The Electrochemical Society (2006-2008), Air Products Faculty Excellence Award (2006); Dupont Young Faculty Award (2006); MIT Presidential Energy Research Council (2005); Visiting Professorship at the University of Bordeaux I, France (2004); Office of Naval Research Young Investigator Award (2003); Atlantic Richfield Career Development Professorship (2002); NSF International Research Fellow Award (2000); Norman Hackerman Young Author Award of The Electrochemical Society (1999); Battery Division Student Research Award of The Electrochemical Society (1997).

Representative Publications of Yang Shao-Horn

1. S. Yuan, J. Peng, B. Cai, Z. Huang, A.T. Garcia-Esparza, D. Sokaras, Y. Zhang, L. Giordano, K. Akkiraju, Y. Zhu, R. Hubner, X. Zou, Y. Roman-Leshkov and Y. Shao-Horn, Tunable Metal-Hydroxide-Organic Frameworks for Catalyzing Oxygen Evolution, *Nature Materials*, 21, 673-680, February 2022.
2. T. Wang, Y. Zhang, B. Huang, B. Cai, R.R. Rao, L. Giordano, S.G. Sun and Y. Shao-Horn, Enhancing the Catalysis of Oxygen Reduction Reaction via Tuning Interfacial Hydrogen Bonds, *Nature Catalysis*, 4, 753-762, September 2021.
3. H. Iriawan, S.Z. Andersen, X. Zhang, B. M. Comer, J. Barrio, P. Chen, A.J. Medford, I.E.L. Stephens, I. Chorkendorff and Y. Shao-Horn, Methods for nitrogen activation by reduction and oxidation, *Nature Reviews Methods Primers*, [1], 56, August 2021.
4. B. Huang, R.R. Rao, S. You, K. H. Myint, Y. Song, Y. Wang, W. Ding, L. Giordano, Y. Zhang, T. Wang, S. Mui, Y. Katayama, J. C. Grossman, A. P. Willard, K. Xu, Y. Jiang and Y. Shao-Horn, Cation- and pH-Dependent Hydrogen Evolution and Oxidation Reaction Kinetics, *Journal of the American Chemical Society Au*, 14, 6030-6040, August 2021.
5. J. Hwang, R.R. Rao, L. Giordano, K. Akkiraju, X.R. Wang, E. Crumlin and Y. Shao-Horn, Regulating oxygen activity of perovskites to promote NO_x oxidation, *Nature Catalysis*, 4, 663-673, July 2021.
6. B. Qiao, S. Mohapatra, J. Lopez, G.M. Leverick, R. Tatara, Y. Shibuya, Y. Jiang, A. France-Lanord, J.C. Grossman, R. Gomez-Bombarelli, J.A. Johnson, and Y. Shao-Horn, Quantitative Mapping of Molecular Substituents to Macroscopic Properties Enables Predictive Design of Oligoethylene Glycol-Based Lithium Electrolytes, *ACS Central Science*, 6, 1115-1128, June 2020.
7. R.R. Rao, M.J. Kolb, L. Giordano, A. F. Pederson, Y. Katayama, J. Hwang, A. Mehta, H. You, J.R. Lunger, H. Zhou, N.B. Halck, T. Vegge, I. Chorkendorff, I.E.L. Stephens, and Y. Shao-Horn, Operando Identification of Site-Dependent Water Oxidation Activity on Ruthenium Dioxide Single-Crystal Surfaces, *Nature Catalysis*, 3, 516-525, May 2020.
8. N. Charles, Y. Yu, L. Giordano, R. Jung, F. Maglia, and Y. Shao-Horn, Towards Establishing Electronic and Phononic Signatures of Reversible Lattice Oxygen Oxidation in Lithium Transition Metal Oxides for Li-Ion Batteries, *Chemistry of Materials*, 32, 5502-5514, May 2020.
9. Y. Zhang, Y. Katayama, R. Tatara, L. Giordano, Y. Yu, D. Fraggedakis, J. Sun, F. Maglia, R. Jung, M.Z. Bazant and Y. Shao-Horn, Revealing Electrolyte Oxidation via Carbonate Dehydrogenation on Ni-based Oxides in Li-ion Batteries by in situ Fourier Transform Infrared Spectroscopy, *Energy and Environmental Science*, 13, 183-199, November 2019.
10. C. Wei, R. R. Rao, J. Peng, B. Huang, I. E. Stephens, M. Risch, Z. J. Xu, and Y. Shao-Horn, Recommended Practices and Benchmark Activity for Hydrogen and Oxygen Electrocatalysis in Water Splitting and Fuel Cells, *Advanced Materials*, 31, 180296, August 2019.
11. B.J. Hopkins, Y. Shao-Horn, and D. P. Hart, Suppressing Corrosion In Primary Aluminum–Air Batteries Via Oil Displacement, *Science*, 362, 658-661 November 2018.
12. J. Hwang, R.R. Rao, L. Giordano, Y. Katayama, Y. Yu, and Y. Shao-Horn, Perovskites in Catalysis and Electrocatalysis, *Science*, 358, 751-756 November 2017.
13. S. Feng, M. Chen, L. Giordano, M. Huang, W. Zhang, C.V. Amanchukwu, R. Anandakathir,

- Y. Shao-Horn, and J.A. Johnson, Mapping a stable solvent structure landscape for aprotic Li–air battery organic electrolytes, *Journal of Materials Chemistry A*, 5, 23987-23998 November 2017.
14. W. Hong, K.A. Stoerzinger, Y.-L. Lee, L. Giordano, A.J.L. Grimaud, A.M. Johnson, J. Hwang, E. Crumlin, W. Yang, Y. Shao-Horn, Charge-transfer-energy-dependent oxygen evolution reaction mechanisms for perovskite oxides, *Energy & Environmental Science*, 10, 2190-2200 October 2017.
 15. L. Giordano, P. Karayaylali, Y. Yu, Y. Katayama, F. Maglia, S. Lux, and Y. Shao-Horn, Chemical Reactivity Descriptor for the Oxide-Electrolyte Interface in Li-Ion Batteries, *Journal of Physical Chemistry Letters*, 8, 3881-3887 August 2017.
 16. A. Grimaud, O. Diaz-morales, B.H. Han, W. T. Hong, Y.L. Lee, L. Giordano, K. A. Stoerzinger, M.T.M. Koper, Y. Shao-Horn, Activating lattice oxygen redox reactions in metal oxides to catalyze oxygen evolution, *Nature Chemistry*, 9, 457-465 May 2017.
 17. J. Bachman, S. Muy, Grimaud, A., H.H. Chang, N. Pour, S. Lux, O. Paschos, F. Maglia, S. Lupart, P. Lamp, L. Giordano and Y. Shao-Horn, Inorganic Solid-State Electrolytes for Lithium Batteries: Mechanisms and Properties Governing Ion Conduction, *Chemical Reviews*, 116, 140-162 January 2016.
 18. D. Kwabi, V.S. Bryantsev, T.P. Batcho, D. Itkis, C.V. Thompson and Y. Shao-Horn, Experimental and Computational Analysis of the Solvent-Dependent $O_2/Li^+-O_2^-$ Redox Couple: Standard Potentials, Coupling Strength and Implications for Lithium-Oxygen Batteries, *Angewandte Chemie International Edition*, 128, 3181-3186 February 2016.
 19. W.T. Hong, K.A. Stoerzinger, B. Mortiz, T.P. Devereaux, W. Yang, and Y. Shao-Horn, Probing $LaMO_3$ Metal and Oxygen Partial Density of States Using X-ray Emission, Absorption, and Photoelectron Spectroscopy, *Journal of Physical Chemistry C*, 119, 2063-2072 2015.
 20. B. Han, C.E. Carlton, A. Kongkanand, R.S. Kukreja, B.R.C. Theobald, L. Gan, R. O'Malley, P. Strasser, F.T. Wagner, and Y. Shao-Horn, Record Activity and Stability of Dealloyed Bimetallic Catalysts for Proton Exchange Membrane Fuel Cells, *Energy & Environmental Science*, 8, 258-266 2015.
 21. J. Suntivich, H.A. Gasteiger, N. Yabuuchi, H. Nakanishi, J.B. Goodenough and Y. Shao-Horn, Design Principles for Oxygen Reduction Activity on Perovskite Oxide Catalysts for Fuel Cells and Metal-Air Batteries, *Nature Chemistry*, 3, 546–550 2011.
 22. J. Suntivich, K.J. May, H.A. Gasteiger, J.B. Goodenough and Y. Shao-Horn, A Perovskite Oxide Optimized for Oxygen Evolution Catalysis from Molecular Orbital Principles, *Science*, 334, 1383-1385 2011.
 23. Y. L. Lee, J. Kleis, J. Rossmeisl, Y. Shao-Horn and D. Morgan, Prediction of Solid Oxide Fuel Cell Cathode Activity with First-Principles Descriptors, *Energy & Environmental Science*, 4, 3966-3970 2011.
 24. S. W. Lee, N. Yabuuchi, G.M. Gallant, S. Chen, B.S. Kim, P.T. Hammond and Y. Shao-Horn, High-Power Lithium Batteries from Functionalized Carbon-Nanotube Electrodes, *Nature Nanotechnology*, 5, 531–537 2010.
 25. S. Chen, W.C. Sheng, N. Yabuuchi, P.J. Ferreira, L.F. Allard and Y. Shao-Horn, The Origin of Oxygen Reduction Activity of “Pt₃Co” Nanoparticles: Atomically Resolved Chemical Compositions and Structures, *Journal of Physical Chemistry C*, 113, 1109–1125 2009.
 26. P.J. Ferreira, G.J. la O', Y. Shao-Horn, D. Morgan, R. Makharia, S. Kocho and H. Gasteiger, Instability of Pt/C Electrocatalysts in Proton Exchange Membrane Fuel Cells: A Mechanistic Investigation, *Journal of the Electrochemical Society*, 152, A2256–A2271 2005.

Selected Lectures of Yang Shao-Horn

Professor Shao-Horn has given ~300 invited, keynote and plenary lectures at university seminars, national and international conferences and events.

1. September 2022, Oxygen evolution on Rutile Ruthenium and Iridium Dioxides, **Plenary**, German Physics Society, Regensburg, Germany.
2. June 2022, Towards Net Zero, **Opening Lecture**, The Fischer Symposium, Kloster Seon, Seon, Germany.
3. May 2022, Towards Net Zero, **Karl Wamsler Innovation Award Address**, Technical University of Munich, Munich, Germany.
4. May 2022, Regulating Surface Oxygen Activity to Tune Reaction Kinetics, **Keynote**, 27th North American Catalysis Society Meeting, New York.
5. November 2021, Mitigating Climate Change, CHUK, **100th Anniversary Celebration Lecture**, virtual.
6. October 2021, Addressing Scientific Challenges to Mitigate Climate Change, **Colloquium at Fritz Haber Institute of the Max Planck Society**, Berlin, Germany.
7. April 2021, Towards decarbonizing chemicals and fuels, **Andlinger Center Seminar**, Princeton University, virtual.
8. December 2019, Anonymous but Curious, **FAIL – Inspiring Resilience**, MIT, Cambridge.
9. July 2019, Energy Storage: Current and Future, **Plenary**, NanoKorea, Seoul, Korea.
10. March 2019, Oxygen redox in metal oxides, **Plenary**, IBA, San Diego, CA.
11. September 2018, “Electrocatalysis for Storing Electrons”, **RSC Faraday Medal Address**, Manchester, UK.
12. May 2018, “Energy Outlook 2050”, **Stanford Energy Seminar**, Stanford University, Palo Alto, CA.
13. September 2017, “The Future of Electrochemistry”, **Marvel Lecture**, EPFL, Lausanne, Switzerland.
14. January 2017, “A Grand Challenge: Energy Storage”, **IdeasLab**, World Economics Forum, Davos, Switzerland.
15. August 2016, “Oxygen electrochemistry for Chemical Storage”, **Keynote**, Inauguration of Villum Center for Sustainable Fuels and Chemicals, Denmark.
16. October 2015, “Activating Oxygen Chemistry of Energy Storage”, **BASF Lectureship**, UC Berkeley, CA.
17. March 2015, Oxygen Electrochemistry and Design of Oxides for Clean Energy and Clean Environment, **Keynote**, BASF Energy Symposium for 150 Year Celebration, Ludwigshafen, Germany.
18. August 2014, “Enabling Oxides for Oxygen Electrocatalysis,” **Plenary**, International Society of Electrochemistry, Lausanne Switzerland.
19. July 2014, Design Principles of Oxides for Oxygen Electrocatalysis, **Keynote**, Nano2014, Moscow, Russia.
20. June 2014, “The Solvation Influence on the Oxygen Redox for Rechargeable Li-air Batteries”, **Plenary**, IMLB 2014, Como, Italy.
21. February 2013, Oxygen Electrolysis on Oxides for Clean Energy Applications, **Plenary**, Zing Conference on Electrochemistry, Canary Islands, Spain.
22. February 2012, “Design Principles for Oxygen Reduction and Evolution on Oxide Catalysts,” **Plenary**, APS March National Meeting, Boston, MA.

Full Publications of Yang Shao-Horn

Professor Shao-Horn and coworkers have published ~390 peer-reviewed archival journal publications.

1. G. Bradford, J. Lopez, J. Ruza, M.A. Stolberg, R. Osterude, J.A. Johnson, R. Gomez-Bombarelli and Y. Shao-Horn, Chemistry-Informed Machine Learning for Polymer Electrolyte Discovery, *ACS Central Science*, [DOI:10.1021/acscentsci.2c01123], January 2023.
2. Y. G. Zhu, J.-H. Fang and Y. Shao-Horn, High Specific-Capacity Al-Graphite Dual-Ion Batteries, *Journal of the Electrochemical Society*, 170, 020503, February 2023.
3. J. Peng, J.J. Giner-Sanz, L. Giordano, W.P. Mounfield, G.M. Leverick, Y. Yu, Y. Roman-Leshkov, and Y. Shao-Horn, Design Principles for Transition Metal Nitride Stability and Ammonia Generation in Acid, *Joule*, 7, 150-167, December 2022.
4. Y. G. Zhu, G. Leverick, A. Accogli, K. Gordiz, Y. R. Zhang, and Y. Shao-Horn, A High-Rate and High-Efficiency Molten-Salt Sodium-Oxygen Battery, *Energy & Environmental Science*, 15, 4636-4646, September 2022.
5. S. Gong, S. Wang, T. Xie, W.H. Chae, R. Liu, Y. Shao-Horn and J.C. Grossman, Calibrating DFT Formation Enthalpy Calculations by Multifidelity Machine Learning, *Journal of the American Chemical Society* Au, 2, 1964-1977, September 2022.
6. S.I. Etkind, J. Lopez, Y. G. Zhu, J. H. Fang, W. J. Ong, Y. Shao-Horn, and T. M. Swager, Thianthrene-Based Bipolar Redox-Active Molecules toward Symmetric All-Organic Batteries, *ACS Sustainable Chemistry & Engineering*, 10, 11739-11750, August 2022.
7. J. Peng, L. Giordano, T. C. Davenport, and Y. Shao-Horn, Stability Design Principles of Manganese-Based Oxides in Acid, *Chemistry of Materials*, 34, 7774-7787, August 2022.
8. J. Peng, D. Schwalbe-Koda, K. Akkiraju, T. Xie, L. Giordano, Y. Yu, C. J. Eom, J.R. Lunger, D.J. Zheng, R.R. Rao, S. Muy, J.C. Grossman, K. Reuter, R. Gómez-Bombarelli and Y. Shao-Horn, Human- and Machine-Centred Designs of Molecules and Materials for Sustainability and Decarbonization, *Nature Reviews Materials*, 7, 2058-8437, August 2022.
9. T.N. Narayanan, G. He, E. Gencer, Y. Shao-Horn and D.S. Mallapragada, Role of Liquid Hydrogen Carriers in Deeply Decarbonized Energy Systems, *ACS Sustainable Chemical Engineering*, 10, 10758-10780, August 2022.
10. Y.G. Zhu, G. Leverick, L. Giordano, S. Feng, Y. Zhang, Y. Yu, R. Tatara, J.R. Lunger and Y. Shao-Horn, Nitrate-mediated four-electron oxygen reduction on metal oxides for lithium-oxygen batteries, *Joule*, 6, 1887-1903, August 2022.
11. S. Gong, T. Xie, Y. Shao-Horn, R. Gomez-Bombarelli and J.C. Grossman, Examining graph neural networks for crystal structures: limitation on capturing periodicity, arXiv preprint, [arXiv:2208.05039], August 2022.
12. T. Xie, H.-K. Kwon, D. Schweigert, S.Gong, A. France-Lanord, A. Khajeh, E. Crabb, M. Puzon, C. Fajardo, W. Powelson, Y. Shao-Horn and J.C. Grossman, A cloud platform for automating and sharing analysis of raw simulation data from high throughput, arXiv preprint, [arXiv:2208.01692], August 2022.
13. M. Burke Stevens, M. Anand, M.E. Kreider, E.K. Prince, J. Zamara Zeledon, L. Wang, J. Peng, H. Li, J.M. Gregoire, J. Hummelshoj, T.F. Jaramillo, H. Jia, J.K. Norskov, Y. Roman-Leshkov, Y. Shao-Horn, B.D. Storey, S. K. Suram, S.B. Torrisi and J.K. Montoya, New challenges in oxygen reduction catalysis: a consortium retrospective to inform future research, *Energy & Environmental Science*, 15, 3775-3794, July 2022.

14. T. Xie, A. France-Lanord, Y. Wang, J. Lopez, M.A. Stolberg, M. Hill, G.M. Leverick, R. Gomez-Bombarelli, J.A. Johnson, Y. Shao-Horn and J.C. Grossman, Accelerating amorphous polymer electrolyte screening by learning to reduce errors in molecular dynamics simulated properties, *Nature Communications*, 13, 3415, June 2022.
15. S. Yuan, J. Peng, Y. Zhang, D.J. Zheng, S. Bagi, T. Wang, Y. Roman and Y. Shao-Horn, Tuning the Catalytic Activity of Fe-Phthalocyanine-Based Catalysts for the Oxygen Reduction Reaction by Ligand Functionalization, *ACS Catalysis*, 12, 7278-7287, June 2022.
16. Z. Ren, L. Ruan, L. Yin, K. Akkiraju, L. Giordano, Z. Liu, S. Li, Z. Ye, S. Li, H. Yang, Y. Wang, H. Tian, G. Liu, Y. Shao-Horn and G. Han, Surface Oxygen Vacancies Confined by Ferroelectric Polarization for Tunable CO Oxidation Kinetics, *Advanced Materials*, 34, 2202072, May 2022.
17. J.J. Giner-Sanz, G.M. Leverick, L. Giordano, V. Perez-Herranz and Y. Shao-Horn, Alkali Metal Salt Interference on the Salicylate Method for Quantifying Ammonia from Nitrogen Reduction, *Electrochemical Society Advances*, 1, 024501, May 2022.
18. M. Chatenet, B.G. Pollet, D.R. Dekel, F. Diongi, J. Deseure, P. Millet, R.D. Braatz, M.Z. Bazant, M. Eikerling, I. Staffell, P. Balcombe, Y. Shao-Horn, and H. Schafer, Water Electrolysis: from textbook knowledge to the latest scientific strategies and industrial developments, *Chemical Society Reviews*, 51, 4583-4762, May 2022.
19. G. Leverick, Y. G. Zhu, S. Lohmar, F. Barde, S. Cotter and Y. Shao-Horn, Six-Electron Reduction for LiIO_3 to LiOH in Aprotic Solvents and Implications for Li-O_2 Batteries, *Journal of Physical Chemistry C*, 126, 8256-8267, May, 2022.
20. J.R. Lunger, N. Lutz, J. Peng, M. Bajdich and Y. Shao-Horn, Cation-Dependent Multielectron Kinetics of Metal Oxide Splitting, *Chemistry of Materials*, 34, 3872-3881, April 2022.
21. Y. Xu, K. Dong, Y. Jie, P. Adelhelm, Y. Chen, L. Xu, P. Yu, J. Kim, Z. Kochovski, Z. Yu, W. Li, J. LeBeau, Y. Shao-Horn, R. Cao, S. Jiao, T. Cheng, I. Manke and Y. Lu, Promoting Mechanistic Understanding of Lithium Deposition and Solid-Electrolyte Interphase (SEI) Formation Using Advanced Characterization and Simulation Methods: Recent Progress, Limitations, and Future Perspectives, *Advanced Energy Materials*, 12, 2200398, March 2022.
22. S.B. Scott, J.E. Sorensen, R.R. Rao, C. Moon, J. Kibsgaard, Y. Shao-Horn and I. Chorkendorff, The low overpotential regime of acidic water oxidation part II: Trends in metal and oxygen stability numbers, *Energy and Environmental Science*, 15, 1988-2001, March 2022.
23. S.B. Scott, R.R. Rao, C. Moon, J.E. Sorensen, J. Kibsgaard, Y. Shao-Horn and I. Chorkendorff, The low overpotential regime of acidic water oxidation part I: The importance of O_2 detection, *Energy and Environmental Science*, 15, 1977-1987, March 2022.
24. S. Yuan, J. Peng, B. Cai, Z. Huang, A.T. Garcia-Esparza, D. Sokaras, Y. Zhang, L. Giordano, K. Akkiraju, Y. Zhu, R. Hubner, X. Zou, Y. Roman-Leshkov and Y. Shao-Horn, Tunable Metal-Hydroxide-Organic Frameworks for Catalyzing Oxygen Evolution, *Nature Materials*, 21, 673-680, February 2022.
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