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/phononic structures 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, CO_2 or nitrogen, to rechargeable lithium-ion/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. The research is highly interdisciplinary and involving close collaborations 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 IrO_2 (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-oxygen covalency and activating surface oxygen sites points to a new direction to increase oxide activity and stability.

Recently, tuning surface oxygen activity using electronic structure has been applied in the design of positive electrode materials 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). Increasing metal-oxygen covalency enhances dissociative adsorption of carbonate molecules on surface oxygen sites, which generates protic species to de-fluorinate electrolyte salt, and produce dehydrogenated organic species (Zhang et al., EES 2019). New electrolyte solvents resistant to oxidative dehydrogenation were designed and used to show excellent cycling of nickel-rich positive electrodes as well as lithium (Xue et al. Nature Energy 2021).

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 (Han et al. 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 (Muy et al. Chem Review 2016, EES 2018 and JACS 2018). Such school of thoughts are being used to search and discover new solid state electrolytes (Muy et al. 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 and Bradford et al., ACS Central Science 2023).

More recently, Professor Shao-Horn and collaborators have shown that tuning non-convalent 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 N_2 and CO_2 reduction to make fuels from electricity from Solar/Wind.

Professor Shao-Horn is a member of National Academy of Engineering, and is among top five most cited female researchers in chemistry in the world, and *Highly Cited Researchers* (Thomson Reuters) based on ~420 archival journal papers (~77,500 citations and h-index of 133 on Google Scholar) and ~350 invited, keynote and plenary lectures in academia (e.g. Marvel Lecture 2017 and Cardona Lecture 2019), at industrial events (e.g., BASF 150 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 (~40) 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. In addition, she is serving on the Board of Directors and advisory boards of private/public organizations including SLAC/SUNCAT, ENSUS research chair at Mohammed VI Polytechnic University (Morocco), Fritz Haber Institute of Max Planck Society (Germany) and Wallenberg Initiative Materials Science for Sustainability (Sweden). Moreover, Professor Shao-Horn serves on advisory boards of leading journals including the Journal of Physical Chemistry in ACS, and 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

Otto Warburg Prize of the University of Bayreuth (2024); International Award for Lithium Batteries (IALB-2023); Best Female Scientists (https://research.com/scientists-rankings/best-female-scientists); Adjunct Senior Scientist at Columbia University (2023-2024); Hans Fischer Senior Fellow of the Technical University of Munich (2022-2026); J.R. East Professor of Engineering (2021-present); 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); Faraday Medal from Royal Society of Chemistry (2018); 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), Air Products Faculty Excellence Award (2006); Dupont Young Faculty Award (2006); MIT Presidential Energy Research Council (2005); 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. Han, P. Wen, H. Wang, Y. Zhou, Y. Gu, L. Zhang, Y. Shao-Horn, X. Lin, and M. Chen, Sequencing Polymers to Enable Solid-State Lithium Batteries, *Nature Materials*, 22, 1515-1522, December 2023.
2. 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*, 9, 206-216, January 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. 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.
6. 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.
7. 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.
8. B. Huang, R.R. Rao, S. You, K. H. Myint, Y. Song, Y. Wang, W. Ding, L. Giordano, Y. Zhang, T. Wang, S. Muy, 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.
9. 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.
10. 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.
11. 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.
12. 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.
13. 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.
14. 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.
15. 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.
16. 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.
17. 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.
18. 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.
19. 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.
20. 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.
21. 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.
22. 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.
23. 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.
24. 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.
25. 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.
26. 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.
27. 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.
28. 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.

29. S. Chen, W.C. Sheng, N. Yabuuchi, P.J. Ferreira, L.F. Allard and Y. Shao-Horn, The Origin of Oxygen Reduction Activity of "Pt_3Co" Nanoparticles: Atomically Resolved Chemical Compositions and Structures, *Journal of Physical Chemistry C*, 113, 1109–1125 2009.
30. P.J. Ferreira, G.J. la O', Y. Shao-Horn, D. Morgan, R. Makharia, S. Kocha 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 ~350 invited, keynote and plenary lectures at university seminars, national and international conferences and events.

1. April 2024, Electrochemistry Renaissance for Climate Action, **Materials Science Seminar**, Boston University, MA.
2. March 2024, Understanding Electrolytes to Enable Advanced Batteries, **Opening Lecture**, Munch Battery Discussion, Munich, Germany.
3. February 2024, Electrochemistry Renaissance for Climate Action, **Initiative for Computational Catalysis of Simons Foundation**, Flatiron Institution, New York City, NY.
4. November 2023, Understanding Electrolytes to Enable Advanced Batteries, **IALB-Award Address**, ABAA-14, Ho Chi Minh City, Vietnam.
5. November 2023, Electrochemistry Renaissance for Climate Action, **Chemistry Seminar**, MIT Chemistry Department, Cambridge, MA.
6. August 2023, Energy Storage for Climate Action, **Opening Lecture**, SUNCAT Summer School, Stanford University, Stanford, CA.
7. September 2022, Oxygen evolution on Rutile Ruthenium and Iridium Dioxides, **Plenary**, German Physics Society, Regensburg, Germany.
8. June 2022, Towards Net Zero, **Opening Lecture**, The Fischer Symposium, Kloster Seeon, Seeon, Germany.
9. May 2022, Towards Net Zero, **Karl Wamsler Innovation Award Address**, Technical University of Munich, Munich, Germany.
10. May 2022, Regulating Surface Oxygen Activity to Tune Reaction Kinetics, **Keynote**, 27th North American Catalysis Society Meeting, New York City, NY.
11. November 2021, Mitigating Climate Change, CHUK, **100th Anniversary Celebration Lecture**, virtual.
12. October 2021, Addressing Scientific Challenges to Mitigate Climate Change, **Colloqium at Fritz Haber Institute of the Max Planck Society**, Berlin, Germany.
13. April 2021, Towards decarbonizing chemicals and fuels, **Andlinger Center Seminar**, Princeton University, virtual.
14. December 2019, Anonymous but Curious, **FAIL – Inspiring Resilience**, MIT, Cambridge.
15. July 2019, Energy Storage: Current and Future, **Plenary**, NanoKorea, Seoul, Korea.
16. March 2019, Oxygen redox in metal oxides, **Plenary**, IBA, San Diego, CA.
17. September 2018, "Electrocatalysis for Storing Electrons", **RSC Faraday Medal Address**, Manchester, UK.
18. May 2018, "Energy Outlook 2050", **Stanford Energy Seminar**, Stanford University, Palo Alto, CA.
19. September 2017, "The Future of Electrochemistry", **Marvel Lecture**, EPFL, Lausanne, Switzerland.
20. January 2017, "A Grand Challenge: Energy Storage", **IdeasLab**, World Economics Forum, Davos, Switzerland.
21. August 2016, "Oxygen electrochemistry for Chemical Storage", **Keynote**, Inauguration of Villum Center for Sustainable Fuels and Chemicals, Denmark.
22. October 2015, "Activating Oxygen Chemistry of Energy Storage", **BASF Lectureship**, UC Berkeley, CA.

23. March 2015, Oxygen Electrochemistry and Design of Oxides for Clean Energy and Clean Environment, **Keynote**, BASF Energy Symposium for 150 Year Celebration, Ludwighafen, Germany.
24. August 2014, "Enabling Oxides for Oxygen Electrocatalysis," **Plenary**, International Society of Electrochemistry, Lausanne Switzerland.
25. July 2014, Design Principles of Oxides for Oxygen Electrocatalysis, **Keynote**, Nano2014, Moscow, Russia.
26. June 2014, "The Solvation Influence on the Oxygen Redox for Rechargeable Li-air Batteries", **Plenary**, IMLB 2014, Como, Italy.
27. February 2013, Oxygen Electrolysis on Oxides for Clean Energy Applications, **Plenary**, Zing Conference on Electrochemistry, Canary Islands, Spain.
28. 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 ~420 peer-reviewed archival journal publications.

1. H. Xu, D. Zheng, H. Iriawan, J. Fang, J. Kim, X. Wang, Y. Román-Leshkov, J. Li, and Y. Shao-Horn, A Cobalt-Platinum-Ruthenium System for Acidic Methanol Oxidation, *Chemistry of Materials*, 2024.
2. D. Chipoco Haro, L. Barrera, H. Iriawan, A. Herzog, N. Tian, A. Medford, Y. Shao-Horn, F. Alamgir, and M. Hatzell, Electrocatalysis for Inorganic and Organic Waste Nitrogen Conversion, *ACS Catalysis*, 14, 13, 9752-9775, 2024.
3. J. Halldin Stenlid, P. Žguns, D. Vivona, A. Aggarwal, K. Gordiz, Y. Zhang, S. Pathak, M. Bazant, Y. Shao-Horn, A. Vaskin, and J. Lawson, Computational Insights into Electrolyte-Dependent Li-ion Charge-Transfer Kinetics at the Li^xCoO_2 Interface, *ACE Energy Letters,* 9, 3608-3617, 2024.
4. Y. Zhang, D. Fraggedakis, T. Gao, S. Pathak, D. Zhuang, C. Grosu, Y. Samantaray, A. Neto, S. Duggirala, B. Huang, Y. Guang Zhu, L. Giordano, R. Tatara, H. Agarwal, R. Stephens, M. Bazant, and Y. Shao-Horn, Lithium-Ion Intercalation by Coupled Ion-Electron Transfer, *ChemRxiv*, preprint doi:10.26434/chemrxiv-2024-d00cp-v2, 2024.
5. A. Aggarwal, K. Gordiz, A. Baskin, D. Vivona, J. Halldin Stenlid, J. Lawson, J. Grossman, and Y. Shao-Horn, Revealing the Molecular Origin of Driving Forces and Thermodynamic Barriers for Li^+ Ion Transport to Electrode-Electrolyte Interfaces, *ChemRxiv*, preprint doi:10.26434/chemrxiv-2024-hn926, 2024.
6. L. Schofield, B. Paren, R. Macdonald, Y. Shao-Horn, and D. Mallapragada, Dynamic Optimization of Proton Exchange Membrane Water Electrolyzers Considering Usage-Based Degradation, *arXiv*, 2405.06766, 2024.
7. K. Akkiraju, R. Rao, J. Hwang, L. Giordano, X.R. Wang, E. Crumlin, D.S. Weinberger, and Y. Shao-Horn, Regulating Oxygen Activity of Perovskites to Promote Activity and Selectivity for Methanol Oxidation to Formaldehyde, *ACS Catalysis*, 14, 7649-7663, 2024.
8. J. Lunger, J. Karaguesian, H. Chun, J. Peng, Y. Tseo, C.H. Shan, B. Han, Y. Shao-Horn, and R. Gómez-Bombarelli, Towards Atom-Level Understanding of Metal Oxide Catalysts for the Oxygen Evolution Reaction with Machine Learning, *NPJ | Computational Materials*, 10, 80, 2024.
9. S. Kwon, K. Stoerzinger, R. Rao, L. Qiao, W. Goddard III, and Y. Shao-Horn, Facet-Dependent Oxygen Evolution Reaction Activity of IrO_2 from Quantum Mechanics and Experiments, *Journal of the American Chemical Society*, 146, 17, 11719–11725, 2024.
10. S. Yu, H. Yamauchi, J. Kim, B. Huang, H. Xu, D. Zheng, X. Wang, H. Iriawan, D. Menga, and Y. Shao-Horn, CO_2-to-Methanol Electroconversion on a Molecular Cobalt Catalyst Facilitated by Acidic Cations, *Chemrxiv*, preprint doi:10.26434/chemrxiv-2023-20v8p-v2, 2024.
11. D.H. Chung, E. Graham, B. Paren, L. Schofield, Y. Shao-Horn, and D. Mallapragada, Design Space for PEM Electrolysis for Cost-Effective H_2 Production Using Grid Electricity, *Industrial & Engineering Chemistry Research*, 63, 16, 7258-7270, 2024.
12. Z. Wang, J.S. Kang, D. Göhl, P. Paciok, D. Gonçalves, H.K. Lim, D. Zanchet, M. Heggen, Y. Shao-Horn, M. Ledendecker, and Y. Román-Leshkov, Platinum/Tantalum Carbide Core-Shell Nanoparticles with Sub-Monolayer Shells for Methanol and Oxygen Electrocatalysis, *Advanced Energy Materials*, 14, 17, 2304092, 2024.
13. E. Crabb, A. Aggarwal, R. Stephens, Y. Shao-Horn, G. Leverick, and J. Grossman, Electrolyte Dependence of Li^+ Transport Mechanisms in Small Molecule Solvents from Classical Molecular Dynamics, *The Journal of Physical Chemistry B*, 124, 14, 3427-3441, 2024.

14. Y. Chen, D. Zheng, Z. Xu, and Y. Shao-Horn, Best Practices for Oxygen Electrocatalysis, *Nature Sustainability*, 7, 371-374, 2024.
15. J. Velasco Vélez, D. Bernsmeier, R. Mom, P. Zeller, Y. Shao-Horn, B. Roldan Cuenya, A. Knop-Gericke, R. Schögl, and T. Jones, Iridium Oxide Coordinatively Unsaturated Active Sites Govern the Electrocatalytic Oxidation of Water, *Advanced Energy Materials*, 14, 2303407, 2024.
16. R. Liu, G. He, X. Wang, D. Mallapragada, H. Zhao, Y. Shao-Horn, and B. Jiang, A Cross-Scale Framework for Evaluating Flexibility Values of Vattery and Fuel Cell Electric Vehicles, *Nature Communications*, 15, 280, 2024.
17. K.H. Pham, K. Gordiz, J.M. Michelsen, H. Liu, D. Vivona, Y. Shao-Horn, A. Henry, K.A. See, and S.K. Cushing, Many-Body Phonon-Ion Conduction in Solid Electrolyte Driven by THz Modes, *arXiv*, 2305.01632, 2023.
18. M. Stolberg, B. Paren, P. Leon, C. Brown, G. Winter, K. Gordiz, A. Concellón, R. Gómez-Bombarelli, Y. Shao-Horn, and J. Johnson, Lamellar Ionenes with Highly Dissociative, Anionic Channels Provide Low Barriers for Cation Transport, *J. Am. Chem. Soc.*, 145, 16200–16209, 2023.
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