

YANG SHAO-HORN

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Professor Shao-Horn is W.M. Keck Professor of Energy at the Massachusetts Institute of Technology (M.I.T.), as well as Professor of Mechanical Engineering and Materials Science and Engineering. 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 the M.I.T. faculty in 2002.

Professor Shao-Horn's research programs are centered on exploiting chemical/materials physics and physical/materials chemistry principles to understand charge transfer at the solid-gas and solid-liquid interface, which is used to design materials/processes and control the kinetics of (electro)chemical reactions, critical to enable the deployment of clean air and clean energy technologies. Professor Shao-Horn and coworkers have pioneered the use of electronic structure to develop universal guiding principles, and design interfaces with activity, reactivity and stability to enhance function/performance across a number of applications spanning from oxidation of air pollutants, making of sustainable or solar fuels via water splitting, CO₂ or nitrogen reduction (Hwang et al., Science 2017), to charge transfer at the electrode/electrolyte interface of 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, and Density Functional Theory computation. Professor Shao-Horn and her coworkers are highly interdisciplinary and collaborate closely with other leading labs and private sectors in chemical, automotive, and energy industry. 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. Also, Shao-Horn and her collaborators have 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). Recently, 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).

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 ~330 archival journal papers (~48,000 citations and h-index of 102 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 ~90 students and postdoctoral associates at MIT, who are now pursuing successful careers in industry, national research laboratories, and in academia (~30) including faculty positions at 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. Furthermore, she has received honors including the Karl Wamsler Innovation Award from Technical University of Munich, Humbolt Prize, the Faraday Medal from RSC, and Mok Hing Yiu Distinguished Visiting Professorship at the Hong Kong University, and has been elected as Fellow from National Academy of Inventors, the American Association for the Advancement of Science, the Royal Society of Chemistry, International Society of Electrochemistry, and the Electrochemical Society.

Representative Publications of Yang Shao-Horn

1. Qiao, B., 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.
2. Rao, R.R., 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.
3. Charles, N., Y. Yang, 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.
4. Zhang, Y., 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.
5. Wei, C., 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*, 2019, **31**, 180296, January 2019.
6. Hopkins, B.J., Y. Shao-Horn, and D. P. Hart, Suppressing Corrosion In Primary Aluminum–Air Batteries Via Oil Displacement, *Science*, **362**, 658-661 November 2018.
7. Kuznetsov, D., B. Han, Y. Yu, R.R. Rao, J. Hwang, Y. Román-Leshkov, and Y. Shao-Horn, Tuning of redox transitions via inductive effect in transition metal complexes and oxides and implications in catalyzing oxygen reduction and oxygen evolution, *Joule*, **2**, 1-20 February 2018.
8. Hwang, J., R.R. Rao, L. Giordano, Y. Katayama, Y. Yu, and Y. Shao-Horn, Perovskites in Catalysis and Electrocatalysis, *Science* **358**, 751-756 November 2017.
9. Feng, S., 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.
10. Tulodziecki, M., G.M. Leverick, C.V. Amanchukwu, Y. Katayama, D.G. Kwabi, F. Bardé, P.T. Hammond and Y. Shao-Horn, The role of iodide in the formation of lithium hydroxide in lithium-oxygen batteries, *Energy & Environmental Science*, **10**, 1828-1842 August 2017.
11. Hong, W., 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.
12. Giordano, L., 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.

13. Grimaud, A., 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.
14. Han, B., K.A. Stoerzinger, V. Tileli, A.D. Gamalski, E.A. Stach, and Y. Shao-Horn, Nanoscale Structural Oscillations in Perovskite Oxides Induced by Oxygen Evolution, *Nature Materials*, 16, 121-126 January 2017.
15. Bachman, J., 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.
16. Kwabi, D., 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.
17. Hong, W.T., M. Risch, K.A. Stoerzinger, A. Grimaud, J. Suntivich, and Y. Shao-Horn, Toward the Rational Design of Non-precious Transition Metal Oxides for Oxygen Electrocatalysis, *Energy & Environmental Science*, 8, 1404-1427 2015.
18. Hong, W.T., 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.
19. Han, B., 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.
20. Grimaud, A., K.J. May, C.E. Carlton, Y.L. Lee, M. Risch, W. Hong, J. Zhou and Y. Shao-Horn, Double Perovskite as a Family of Highly Active Catalysts for Oxygen Evolution in Alkaline Solution, *Nature Communications*, 4, 2439 2013.
21. Suntivich, J., 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. Suntivich, J., 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. Lee, Y. L., 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. Crumlin, E.J, E. Mutoro, S.J. Ahn, G.J. la O', D. N. Leonard, A. Borisevic, M. D. Biegalski, H. M. Christen, Y. Shao-Horn, Oxygen Reduction Kinetics Enhancement on a Hetero-Structured Oxide Surface for Solid Oxide Fuel Cells, *Journal of Physical Chemistry Letters*, 1, 3149-3155 2010.
25. Lee, S.W., 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.
26. Chen, S., 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.
27. Ferreira, P.J., 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 Recent 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. November 2020, Towards identifying active environments in electrocatalysis, **Plenary**, University of Toronto, Canada.
2. September 2020, Materials Challenges for Energy Storage, KAIST Emerging Materials e-Symposium, Korea.
3. July 2020, Oxide Structure and Dynamics for Storing Electrons, Virtual Symposium: **Create a Rechargeable World**, in Honor of Chemistry Nobel Laureate John B. Goodenough's 98th birthday, organized by Wiley Advanced Energy Materials.
4. December 2019, Anonymous but Curious, **FAIL – Inspiring Resilience**, MIT,
5. July 2019, Energy Storage: Current and Future, **Plenary**, NanoKorea, Seoul, Korea.
6. June 2019, Enabling Clean Energy on Demand using Electrochemistry, **Cardona Lecture**, Catalan Institute of Nanoscience and Nanotechnology, Spain.
7. March 2019, Oxygen redox in metal oxides, **Plenary**, IBA, San Diego, CA.
8. October 2018, “Electrified Interface: Challenges and Opportunities”, **Current Challenges in Catalysis**, The Royal Danish Academy of Sciences and Letters, Copenhagen, Denmark.
9. September 2018, “Electrocatalysis for Storing Electrons”, **RSC Faraday Medal Address**, Manchester, UK.
10. May 2018, “Energy Outlook 2050”, **Stanford Energy Seminar**, Stanford University, Palo Alto, CA.
11. October 2017, “Electrochemistry Outlook 2050”, **Nanqiang Lecture**, Xiamen University, Xiamen, China.
12. September 2017, “The Future of Electrochemistry”, **Marvel Lecture**, EPFL, Lausanne, Switzerland.
13. January 2017, “A Grand Challenge: Energy Storage”, **IdeasLab**, World Economics Forum, Davos, Switzerland.
14. August 2016, “Oxygen electrochemistry for Chemical Storage”, **Keynote**, Inauguration of Villum Center for Sustainable Fuels and Chemicals, Denmark.
15. October 2015, “Activating Oxygen Chemistry of Energy Storage”, **BASF Lectureship**, UC Berkeley, CA.
16. March 2015, Oxygen Electrochemistry and Design of Oxides for Clean Energy and Clean Environment, **Keynote**, BASF Energy Symposium for 150 Year Celebration, Ludwigshafen, Germany.
17. August 2014, “Enabling Oxides for Oxygen Electrocatalysis,” **Plenary**, International Society of Electrochemistry, Lausanne Switzerland.
18. July 2014, Design Principles of Oxides for Oxygen Electrocatalysis, **Keynote**, Nano2014, Moscow, Russia.
19. June 2014, “The Solvation Influence on the Oxygen Redox for Rechargeable Li-air Batteries”, **Plenary**, IMLB 2014, Como, Italy.
20. February 2013, Oxygen Electrolysis on Oxides for Clean Energy Applications, **Plenary**, Zing Conference on Electrochemistry, Canary Islands, Spain.
21. 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 ~335 peer-reviewed archival journal publications and is a co-inventor on a number of issued and pending Patents.

1. Yang, Y., P. Karayaylali, D. Sokaras, L. Giordano, R. Kou, C. Sun, F. Maglia, R. Jung, F.S. Gittleston and Y. Shao-Horn, Towards controlling the reversibility of anionic redox in transition metal oxides for high-energy Li-ion positive electrodes, *Energy and Environmental Science*, [DOI: 10.1039/D0EE03765F], February 2021.
2. B. Huang, K.H. Myint, Y. Wang, Y. Zhang, R.R. Rao, J. Sun, S. Muy, Y. Katayama, J. Corchado Garcia, D. Fraggedakis, J.C. Grossman, M.Z. Bazant, K. Xu, A.P. Willard and Y. Shao-Horn, Cation-Dependent Interfacial Structures and Kinetics for Outer-Sphere Electron-Transfer Reactions, *Journal of Physical Chemistry C*, 125, 4397-4411, February 2021.
3. D. Fraggedakis, M. McEldrew, R.B. Smith, Y. Krishnan, Y. Zhang, P. Bai, W. C. Chueh, Y. Shao-Horn and MZ. Bazant, Theory of coupled ion-electron transfer kinetics, *Electrochimica Acta*, 367, 137432, January 2021.
4. S. Khan, J. Hwang, Y. Shao-Horn and K. Varanasi, Catalyst-proximal plastrons enhance activity and selectivity of carbon dioxide electroreduction, *Cell Reports Physical Science*, 2, 100318, January 2021.
5. A.I. Inozemtseva, E.Y. Kataev, A.S. Froloy, M. Amati, L. Gregoratti, K. Beranova, V. Perez Dieste, C. Escudero, A. Federov, A. V. Tarasov, D. Y. Usachov, D. Vyalikh, Y. Shao-Horn, D. M. Itkis, L. V. Yashina, On the catalytic and degradative role of oxygen-containing groups on carbon electrode in non-aqueous ORR, *Carbon*, 176, 632-641, January 2021.
6. W. Zhang, S. Feng, M. Huang, B. Qiao, K. Shigenobu, L. Giordano, J. Lopez, R. Tatara, K. Ueno, K. Dokko, M. Watanabe, Y. Shao-Horn and J.A. Johnson, Molecularly Tunable Polyanions for Single-Ion Conductors and Poly(solvate ionic liquids), *Chemistry of Materials*, 33, 524-534, January 2021.
7. S. Muy, R. Schlem, Y. Shao-Horn, and W.G. Zeier, Phonon-Ion Interactions: Designing Ion Mobility Based on Lattice Dynamics, *Advanced Energy Materials*, [DOI: 10.1002/aenm.202002787], December 2020.
8. Y. Tsuji, S. Sako, K. Nitta, K. Yamamoto, Y. Shao-Horn, Y. Uchimoto and Y. Orikasa, Surface analysis of lanthanum strontium cobalt oxides under cathodic polarization at high temperature through *operando* total-reflection X-ray absorption and X-ray fluorescence spectroscopy, *Solid State Ionics*, 357, 115502, December 2020.
9. Y. Yu, P. Karayaylali, L. Giordano, J. Corchado-García, J. Hwang, D. Sokaras, F. Maglia, R. Jung, F. S. Gittleston, and Y. Shao-Horn, Probing Depth-Dependent Transition-Metal Redox of Lithium Nickel, Manganese, and Cobalt Oxides in Li-Ion Batteries, *ACS Applied Materials and Interfaces*, 12, 55865-55875, December 2020.
10. E. Crabb, A. France-Lanord, G. Leverick, R. Stephens, Y. Shao-Horn, and J.C. Grossman, Importance of Equilibration Method and Sampling for *Ab Initio* Molecular Dynamics Simulations of Solvent-Lithium-Salt Systems in Lithium-Oxygen Batteries, *Journal of Chemical Theory and Computation*, 16, 7255-7266, November 2020.
11. T. Khudiyev, J. T. Lee, J. R. Cox, E. Argentieri, G. Loke, R. Yuan, G. H. Noel, R. Tatara, Y. Yu, F. Logan, J. Joannopoulos, Y. Shao-Horn, and Y. Fink, 100 m Long Thermally Drawn Supercapacitor Fibers with Applications to 3D Printing and Textiles, *Advanced Materials*, 32,

2004971, November 2020.

12. J.J. Giner-Sanz, G. Leverick, V. Perez-Herranz, and Y. Shao-Horn, Salicylate Method for Ammonia Quantification in Nitrogen Electroreduction Experiments: The Correction of Iron III Interference, *Journal of the Electrochemical Society*, **167**, 134519, October 2020.
13. S. Yuan, Li, J. Peng, Y. M. Questell-Santiago, K. Akkiraju, L. Giordano, D.J. Zheng, S. Bagi, Y. Roman-Leshkov, and Y. Shao-Horn, Conversion of Methane in Liquid Fuels – Bridging Thermal Catalysis with Electrocatalysis, *Advanced Energy Materials*, **10**, 2002154, September 2020.
14. T.-H. Shen, L. Spillane, J. Vavra, T. H. M. Pham, Y. Shao-Horn, and V. Tileli, Oxygen Evolution Reaction in $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Co}_{0.8}\text{Fe}_{0.2}\text{O}_{3-\delta}$ Aided by Intrinsic Co/Fe Spinel-Like Surface, *Journal of the American Chemical Society*, **142**, 15876-15833, August 2020.
15. R.R. Rao, M. Tulodziecki, B. Han, M. Risch, A. Abakumov, Y. Yu, P. Karayayalali, M. Gauthier, M. Escudero-Escribano, Y. Orikasa, and Y. Shao-Horn, Reactivity with Water and Bulk Ruthenium Redox of Lithium Ruthenate in Basic Solutions, *Advanced Functional Materials*, **31**, 2002249, July 2020.
16. 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.
17. Y. Zhu, T.N. Narayanan, M. Tulodziecki, H. Sanchez-Casalongue, Q. Horn, L. Meda, Y. Yu, T. Regier, G.H. McKinley, and Y. Shao-Horn, High-energy and high-power Zn-Ni flow batteries with semi-solid electrodes, *Sustainable Energy and Fuels*, **4**, 4076-4085, June 2020.
18. N. Charles, Y. Yang, 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.
19. D. Fraggedakis, T. Gao, T. Zhou, Y. Zhang, Y. Han, R.M. Stephens, Y. Shao-Horn, and M.Z. Bazant, A scaling law to determine phase morphologies during ion intercalation, *Energy and Environmental Sciences*, **13**, 2142-2152, May 2020.
20. T. Kawaguchi, R.R. Rao, J.R. Lunger, Y. Liu, D. Walko, E.A. Karapetrova, V. Komanicky, Y. Shao-Horn, and H. You, Stern layers on RuO_2 (100) and (110) in electrolyte: Surface X-ray scattering studies, *Journal of Electroanalytical Chemistry*, **875**, 114228, May 2020.
21. Rao, R.R., 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.
22. Wang, Y., T. Xie, A. France-Lanord, A. Berkley, J.A. Johnson, Y. Shao-Horn, and J.C. Grossman, Towards Designing Highly Conductive Polymer Electrolyte by Machine Learning Assisted Coarse-Grained Molecular Dynamics, *Chemistry of Materials*, **32**, 4144-4151, April 2020.
23. Han, S., C. Cai, Y. Zhu, Q. Sun, Y. Zhu, H. Li, H. Wang, Y. Shao-Horn, A.X. Sun and M. Gu, Interrogation of the Reaction Mechanism in a Na- O_2 Battery Using *In-Situ* Transmission Electron Microscopy, *ACS Nano*, **14**, 3669-3677, March 2020.
24. Leverick, G., R. Tatara, S. Feng, E. Crabb, A. France-Lanord, M. Tulodziecki, J. Lopez, R.M. Stephens, J.C. Grossman and Y. Shao-Horn, Solvent- and Anion-Dependent Li^+-O_2^- Coupling Strength and Implications on the Thermodynamics and Kinetics of Li- O_2 Batteries, *Journal of*

- Physical Chemistry C, Journal of Physical Chemistry C, 124, 4953-4967, March 2020.
25. Göhl, D., A. Garg, P. Paciok, K.J.J. Mayrhofer, M. Heggen, Y. Shao-Horn, R.E. Dunin-Borkowski, Y. Román-Leshkov and M. Ledendecker, Engineering stable electrocatalysts by synergistic stabilization between carbide cores and Pt shells, *Nature Materials*, 19, 287-291, March 2020.
 26. Gallagher, N., H.Z. Ye, J. Lopez, Y. Zhu, T.V. Voorhis, Y. Shao-Horn and J.A. Johnson, An N-Heterocyclic Carbene Derived Distonic Radical Cation, *Angewandte Chemie*, 59, 3952-3955, March 2020.
 27. Karayaylali, P. Y. Zhang, L. Giordano, Y. Katayama, R. Tatara, Y. Yu, F. Maglia, R. Jung and Y. Shao-Horn, The Role of Diphenyl Carbonate Additive on the Interfacial Reactivity of Positive Electrodes in Li-ion Batteries, *Journal of the Electrochemical Society*, 167, 040522, March 2020.
 28. Li, C.Y., Y. Yu, C. Wang, Y. Zhang, S. Zheng, J.F. Li, F. Maglia, R. Jung, Z.Q. Tian and Y. Shao-Horn, Surface Changes of $\text{LiNi}_x\text{Mn}_y\text{Co}_{1-x-y}\text{O}_2$ in Li-Ion Batteries Using *In Situ* Surface-Enhance Raman Spectroscopy, *Journal of Physical Chemistry C*, 124, 4024-4031, February 2020.
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