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, CO₂ 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 (“e₉” 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 state-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-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
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 N₂ and CO₂ reduction to make fuels from electricity from Solar/Wind.

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.
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EDUCATION
Ph.D. in Metallurgical & Materials Engineering (May 1998)
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Dissertation: The structural stability of transition metal oxides for lithium rechargeable cells.
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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

PROFESSIONAL SOCIETIES
Materials Research Society (1998-present)
American Chemical Society (2002-present)

HONORS and AWARDS
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


28. S. W. Lee, N. Yabuuchi, G.M. Gallant, S. Chen, B.S. Kim, P.T. Hammond and Y. Shao-Horn,


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. September 2022, Oxygen evolution on Rutile Ruthenium and Iridium Dioxides, Plenary, German Physics Society, Regensburg, Germany.
3. May 2022, Towards Net Zero, Karl Wamsler Innovation Award Address, Technical University of Munich, Munich, Germany.
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.
Full Publications of Yang Shao-Horn

Professor Shao-Horn and coworkers have published ~410 peer-reviewed archival journal publications.

Ammonia Generation in Acid, Joule, 7, 150-167, December 2022.
41. 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
54. P. Pascual-Sebastian, Y. Shao-Horn and M. Escudero-Escribano, Toward understanding the role of the electric double layer structure and electrolyte effects on well-defined interfaces for electrocatalysis, Current Opinion in Electrochemistry, 32, 1008918, December 2021.


91. T.-H. Shen, L. Spillane, J. Vavra, T. H. M. Pham, Y. Shao-Horn, and V. Tileli, Oxygen Evolution Reaction in Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-δ} Aided by Intrinsic Co/Fe Spinel-Like Surface, Journal of the American Chemical Society, 142, 15876-15833, August 2020.
96. D. Fraggedakis, T. Gao, T. Zhou, Y. Zhang, Y. Han, R.M. Stephens, Y. Shao-Horn, and M.Z.


fluorosulfonyl” electrolyte for 4V-class lithium-metal batteries, Energy and Environmental Science, 13, 212-220, January 2020.


121. Giordano, L., T.M. Østergaard, S. Muy, Y. Yu, N. Charles, S. Kim, Y. Zhang, F. Maglia, R.


200. Lee, D., Y-L. Lee, X.R. Wang, D. Morgan, and Y. Shao-Horn, Enhancement of oxygen surface exchange on epitaxial La0.4Sr0.6Co0.2Fe0.8O3-δ thin films using advanced heterostructured oxide interface engineering, MRS Communications, 6, 204-209 September 2016.


205. Geary, T., D. Lee, Y. Shao-Horn, and S. Adler, Nonlinear Impedance Analysis of La0.4Sr0.6Co0.2Fe0.8O3-δ Thin Film Oxygen Electrodes, Journal of the Electrochemical Society, 163, F1107-F1114 July 2016.

206. Xie, W., Y-L. Lee, Y. Shao-Horn, and D. Morgan, Oxygen Point Defect Chemistry in Ruddlesden-Popper Oxides (La1-xSr)xMO3+x/2(M=Co, Ni, Cu), The Journal of Physical Chemistry Letters, 7, 1939-1944 May 2016.


27. Lee, D., Y.L. Lee, A. Grimaud, W.T. Hong, M.D. Biegalski, D. Morgan, and Y. Shao-Horn, Enhanced Oxygen Surface Exchange Kinetics and Stability on Epitaxial L$\text{a}$$_{0.8}$Sr$\text{f}$$_{0.2}$CoO$_3$ Thin Films by L$\text{a}$$_{0.8}$Sr$_{0.2}$MnO$_3$ Decoration, Journal of Physical Chemistry C, 118, 14326-14334 June 2014.


30. Lee, D., Y.L. Lee, A.J.L. Grimaud, W. Hong, M. Biegalski, D. Morgan, and Y. Shao-Horn, Strontium Influence on the Oxygen Electrocatalysis of L$_{2-x}$Sr$_x$NiO$_{4+\delta}$ (0.0$\leq$x$\leq$1.0) Thin Films, Journal of Materials Chemistry A, 2, 6480-6487 May 2014.


34. Risch, M., K.A. Stoerzinger, S. Maruyama, W.T. Hong, I. Takeuchi, and Y. Shao-Horn, L$_{0.8}$Sr$_{0.2}$MnO$_3$ Decorated with Ba$_{0.5}$Sr$_{0.5}$Co$_{0.5}$Fe$_{0.5}$O$_3$-δ: A Bi-functional Surface for Oxygen Electrocatalysis with Enhanced Stability and Activity, Journal of the American Society, 136, 5229-5232 April 2014.


Oriented Epitaxial La$_2$NiO$_{4+\delta}$ Thin Films at Elevated Temperatures, Journal of Physical Chemistry C, 117, 18789-18795, September 2013.


300. Quinlan, R.A., Y.-C. Lu, Y. Shao-Horn, and A.N. Mansour, XPS Studies of Surface Chemistry Changes of LiNi$_{0.5}$Mn$_{0.5}$O$_2$ Electrodes During High-Voltage Cycling, Journal of the Electrochemical Society, 160, A669-A677 February 2013.
305. Carlton, C.E., C.A. Kuryak, W.-S. Liu, Z. Ren, G. Chen and Y. Shao-Horn, Disordered Stoichiometric Nanorods and Ordered Off-Stoichiometric Nanoparticles in N-Type Thermoelectric Bi$_2$Te$_{2.7}$Se$_{0.3}$, Journal of Applied Physics, 112, 093518 November 2012.

313. Harding, J., Y-C. Lu, Y. Tsukada and Y. Shao-Horn, Evidence of Catalyzed Oxidation of Li$_2$O$_2$ for Rechargeable Li-Air Battery Applications, Physical Chemistry Chemical Physics, 14, 10540-10546 June 2012.


340. Yabuuchi, N., Y.C. Lu, A.N. Mansour, S. Chen, and Y. Shao-Horn, The Influence of Heat-Treatment Temperature on the Cation Distribution of LiNi\textsubscript{0.5}Mn\textsubscript{0.5}O\textsubscript{2} and Its Rate Capability in Lithium Rechargeable Batteries, Journal of the Electrochemical Society, 158, A192–A200 January 2011.


374. Yabuuchi N., S. Kumar, H.H. Li, Y.T. Kim, and Y. Shao-Horn, Changes in the Structural and Transport Properties of Layered O3 Li$_{1/2}$Ni$_{0.5}$Mn$_{0.5}$O$_2$ during Electrochemical Cycling to High Voltages, Journal of the Electrochemical Society, 154, A566–A578 June 2007.

375. Li, H.H., N. Yabuuchi, Y.S. Meng, S. Kumar, J. Bréger, C.P. Grey, and Y. Shao-Horn, Structural Changes of Li$_{1/2}$Ni$_{0.5}$Mn$_{0.5}$O$_2$ During Electrochemical Cycling to High Voltages: An Electron Diffraction Study, Chemistry of Materials, 19, 2551–2565 April 2007.


381. Breger, J., Y.S. Meng, Y. Hinuma, S. Kumar, Y. Shao-Horn, G. Ceder, and C.P. Grey, The Effect of High Voltages on the Structure and Electrochemistry of Li(NiMn)$_{0.5}$O$_2$; A Joint Experimental and Theoretical Study, Chemistry of Materials, 18, 4768–4781 August 2006.


386. Meng, Y.S., G. Ceder, C.P. Grey, W.S. Yoon, M. Jiang, J. Bréger, and Y. Shao-Horn, Cation Ordering in Layered O3 Li[$\text{Ni}_{1/3}$Li$_{2/3}$xMn$_{1/3}$x]O$_2$ (0 < x < 1/2) Compounds, Chemistry of Materials, 17, 2386–2394 March 2005.


Full Patents and Patent Applications of Yang Shao-Horn


5. Shao-Horn, Yang; Lee, Seung, Woo; Hammond-Cunningham, Paula; Yabuuci, Naoaki. "Layer-By-Layer Assemblies Of Carbon-Based Nanostructures And Their Applications In Energy Storage And Generation Devices". China Serial No. 200980131862.5, Filed August 14, 2009. Publication Number: CN102171870. Published Application


11. Amanchukwu, Chibueze; Shao-Horn, Yang; Ma, Sang Bok; Khiterer, Mariya; Hammond-Cunningham, Paula; Rye, Young-Gyoon. "Stable Electrolyte For Lithium Air Battery And Lithium Air Battery Including The Same", US Serial No. 14/949498, Filed November 23,
2015, Issued April 9, 2019

12. Amanchukwu, Chibueze; Shao-Horn, Yang; Ma, Sang Bok; Khiterer, Mariya; Hammond-Cunningham, Paula; Rye, Young-Gyoong. "Polyacrylate Electrolyte For Li-Air Battery", Korea (south) Serial No. 10-2016-0017768, Filed February 16, 2016. Pending


22. Hwang, Jonathan; Khan, Sami; Shao-Horn, Yang; Varanasi, Kripa. “A Method to Suppress Hydrogen Evolution and Increase Hydrocarbon Generation during Electrochemical Reduction
of CO\textsubscript{2} by Trapping CO\textsubscript{2} Bubbles on Hydrophobic Surfaces Near the Catalyst”, US Serial No. 62/858824, Filed November 28, 2018. Pending


24. Feng, Shuting; Giordano, Livia; Huang, Mingjun; Johnson, Jeremiah; Kim, Tae Young; Shao-Horn, Yang; Zhang, Wenxu. “Polymer Compound, Film Compromising the Same, and Lithium Air Battery Comprising the Film”, Korea (south) Serial No. 10-2019-0153008, Filed January 31, 2019. Pending


26. Feng, Shuting; Giordano, Livia; Huang, Mingjun; Johnson, Jeremiah; Kim, Tae Young; Shao-Horn, Yang; Zhang, Wenxu. “Polymer Compound, Film Compromising the Same, and Lithium Air Battery Comprising the Film”, Korea (south) Serial No. 10-2019-0153008, Filed January 31, 2019. Pending


34. Shao-Horn, Yang; Roman-Leshkov, Yuriy; Peng, Jiayu; “Transition Metal Nitrides As Solid Carriers For Ammonia Storage”, Patent Cooperation Treaty application no. PCT/US/2021/045545, Filed August 11, 2021. Pending


