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A combined ionic Lewis acid descriptor and machine-learning approach to prediction of efficient oxygen reduction electrodes for ceramic fuel cells

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Improved, highly active cathode materials are needed to promote the commercialization of ceramic fuel cell technology. However, the conventional trial-and-error process of material design, characterization and testing can make for a long and complex research cycle. Here we demonstrate an experimentally validated machine-learning-driven approach to accelerate the discovery of efficient oxygen reduction electrodes, where the ionic Lewis acid strength (ISA) is introduced as an effective physical descriptor for the oxygen reduction reaction activity of perovskite oxides. Four oxides, screened from 6,871 distinct perovskite compositions, are successfully synthesized and confirmed to have superior activity metrics. Experimental character- ization reveals that decreased A-site and increased B-site ISAs in perovskite oxides considerably improve the surface exchange kinetics. Theoretical calculations indicate such improved activity is mainly attributed to the shift of electron pairs caused by polarization distribution of ISAs at sites A and B, which greatly reduces oxygen vacancy formation energy and migration barrier.
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