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Probing for cationic dopants in lanthanum manganite for solid oxide fuel cell applications SRIDEVI KRISHNAN, VINIT SHARMA, Material Science and Engineering, Institute of Materials Science, University of Connecticut, Storrs, MANOJ K MAHAPATRA, PRABHAKAR SINGH, Material Science and Engineering, Center for Clean Energy Engineering, University of Connecticut, Storrs, RAMPI RAMPRASAD, Material Science and Engineering, Institute of Materials Science, University of Connecticut, Storrs — Solid oxide fuel cells (SOFC) are an efficient source of clean energy. Long-term stability of SOFC cathodes is desired along with thermophysical characteristics. Sr doped $LaMnO_3$ is one of the active material for this application. A suitable choice of the dopant has a significant influence on the stability and performance of the cathode material at elevated operating temperature. Using first principles computations, we compare the stability of the $LaMnO_3$ host for a range of cationic dopants including alkali, alkaline earth metals, 3d, 4d and 5d transition metal elements in the absence and presence of an oxygen vacancy. The stability of doped $LaMnO_3$ against decomposition to various combinations of metals and oxides is assessed using a linear programming based algorithm, and the oxygen vacancy promoters are identified. Properties of the dopants like the ionic radius, oxidation state, magnetic moment and Mendeleev number are correlated with their stability in the host. Employing these as feature vectors, feature selection methods are used to identify the most promising ones to be used for regression and classification problems. Using supervised learning approaches stability of the dopant in the host is predicted for test sets.

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