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**Pressure-temperature surface phase diagrams of $LaMnO_3$ surfaces in oxidative environments from first principles based kinetic Monte Carlo simulations**[1] GHANSHYAM PILANIA, R. RAMPRASAD, University of Connecticut — Perovskite oxide surfaces catalyze many important oxidation reactions. They are also promising for oxygen ion conducting cathode materials in solid oxide fuel cells and efficient catalytic components for removal of $NO_x$ gases in auto exhausts. Oxygen interaction with perovskite surfaces is of central importance in all such above mentioned technologically relevant examples. Here, we have employed first-principles based kinetic Monte Carlo (kMC) simulations to investigate the relative stability of the clean as well as molecular and atomic oxygen covered $LaMnO_3$ surfaces over a vast range of temperatures and oxygen partial pressures. The energetics as well as the activation energies of various surface reactions (adsorption, desorption, surface dissociation, and the surface diffusion of molecular and atomic oxygen) were computed and used in large-scale kMC simulations to predict the surface oxygen content and configuration at various combinations of temperature and pressure, thereby yielding a surface phase diagram. Owing to the state-of-the-art theory, algorithms and computations employed, these results are believed to represent the real situation with high fidelity. The phase boundaries as predicted by our kMC simulations are identified to be the catalytically active regions.

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