

Showcasing research from Computational NanoPhysics Laboratory, Department of Physics, Kyung Hee University, Korea and Electron Microscopy & Spectroscopy Laboratory, Department of Materials Science and Engineering, Seoul National University, Korea.

Effects of paramagnetic fluctuations on the thermochemistry of MnO(100) surfaces in the oxygen evolution reaction

This work investigates the effects of paramagnetic fluctuations on the thermochemistry of MnO(100) surfaces in the oxygen evolution reaction. Paramagnetic fluctuations enhance charge transfer from a surface metal ion to the reaction intermediates, significantly influencing the thermochemistry of transition metal oxide surfaces. This work suggests that magnetic fluctuations should be considered when quantitatively investigating the free energy diagram of chemical reactions occurring on oxide surfaces.



