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Understanding Iron-based catalysts with efficient Oxygen reduction activity from first-principles calculations HASNAIN HAFIZ, B. BARBIELLINI, Q. JIA, Northeastern U., U. TYLUS, Northeastern U. and LANL, K. STRICKLAND, A. BANSIL, S. MUKERJEE, Northeastern U. — Catalysts based on Fe/N/C clusters can support the oxygen-reduction reaction (ORR) without the use of expensive metals such as platinum. These systems can also prevent some poisonous species to block the active sites from the reactant. We have performed spin-polarized calculations on various Fe/N/C fragments using the Vienna Ab initio Simulation Package (VASP) code. Some results are compared to similar calculations obtained with the Gaussian code. We investigate the partial density of states (PDOS) of the 3d orbitals near the Fermi level and calculate the binding energies of several ligands. Correlations of the binding energies with the 3d electronic PDOS's are used to propose electronic descriptors of the ORR associated with the 3d states of Fe. We also suggest a structural model for the most active site with a ferrous ion (Fe^{2+}) in the high spin state or the so-called Doublet 3 (D3).

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