

TUNING A METAL-OXO GROUP FOR WATER OXIDATION

Ligands determine the reactivity of metal complexes. We discuss how the metal-oxo group, well-known to activate the C-H bond in alkane hydroxylation catalysis, might be tuned into a suitable catalyst for the water oxidation reaction by the choice of ligand framework. Ligand field considerations indicate preference dictated by the nature of the metal, the nature of the ligand donor atoms and the overall charge of the complex. A verification is provided by DFT calculations on a series of iron(IV)oxo (ferryl) complexes which give a singularly low transition state energy barrier for O-O coupling of the oxo group with water oxygen.