

## d-orbital Manifold Controlled Electrocatalyst for Solar Fuel

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Water splitting is a promising step towards sustainable energy schemes. Oxygen evolution reaction requires extremely high overpotential due to slow kinetics. The WOC in PS II, cubical Mn<sub>4</sub>CaO<sub>5</sub> cluster, efficiently catalyzes water oxidation. Inspired by Mn<sub>4</sub>CaO<sub>5</sub> cluster, specific questions that we focus for further applications include how to translate the underlying principles in Mn<sub>4</sub>CaO<sub>5</sub> cluster into synthetic heterogeneous catalysts. Toward this vision, we have been developing a new catalytic platform based on sub-10 nm NPs to bridge the gap between atomically defined biological catalysts, their metalloenzyme counterparts and electrode depositable heterogeneous catalysts. In this approach, local atomic geometry is controlled by nitrogen containing graphitic carbon and heterogeneous atom doping that enhance catalytic activity and selectivity. Additional surface modification by specific ligand allows for the atomic scale tunability to realize unique electronic hybridization.