Illuminating Mechanisms of Water Oxidation Catalysis 50046-ND3

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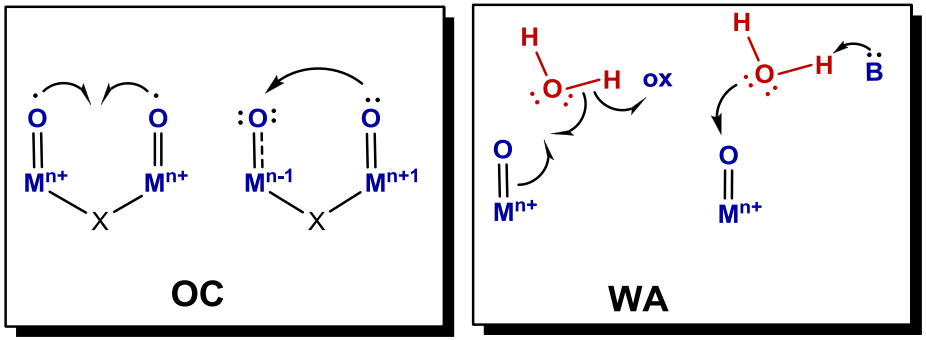
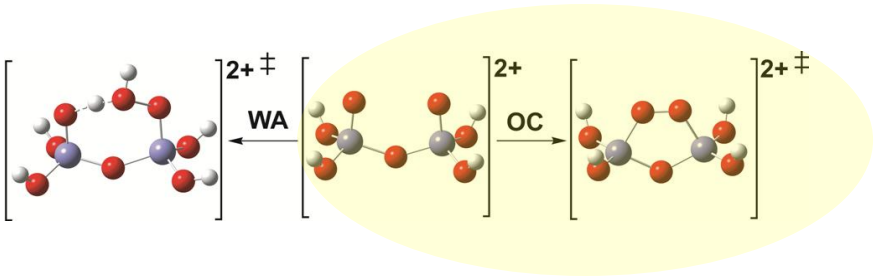
Natural abundance oxygen-18 kinetic isotope effects are being measured and calculated to probe water oxidation mechanisms.

Mechanisms are defined by *intramolecular* oxo-coupling (OC) or *intermolecular* water attack (WA)



Ferrate has been used as a model system where the O-O bond formation step can be isolated and the KIE is shown to be consistent with OC:

$$4[H_3Fe^{VI}O_4]^+ + 8H_3O^+ \rightarrow 4Fe^{3+} + 3O_2 + 18H_2O.$$



Transition states are now being illuminated by modeling changes in bond vibrations in various catalytic systems: