Molecular Water Oxidation Catalysts

Hong-Tao Zhang, Qi-Fa Chen, Fei Xie, Hao-Yi Du, Jing Shi, Ming-Tian Zhang[1]

Center of Basic Molecular Science (CBMS), Department of Chemistry, Tsinghua University, Beijing, 10084, China

E-Mail presenting author: mtzhang@mail.tsinghua.eu.cn

The oxidation of water to oxygen, $2H_2O \rightarrow O_2 + 4H^+ + 4e^-$, is a key step for capturing solar energy in nature. Developing a molecular catalyst that can split water into oxygen and hydrogen is one of the main bottlenecks inhibiting the development of an effective and robust artificial photosynthetic system. The main challenge for catalyst development is that the catalytic process involves accumulative proton coupled electron transfer, multiple bond arrangements and finally the formation of O-O bond. Generally, a high energetic intermediate, $M^{n+}=O$, was essential to O-O bond formation. On the other hand, the formation of high energetic intermediates needs to be avoided as they can reduce the longevity of the WOC and make the operation potential far away from the thermodynamic potential of water oxidation. In PSII, Mn_4Ca cluster distributes charge over multiple metallic centers to avoid charge accumulation on single site and formation of Mn(V) that was proposed as key intermediates for artificial molecular Mn based WOCs.

In this presentation, we will introduce our works on the molecular water oxidation catalysts, mainly focus on the redox active ligand-center PCET assisted water oxidation and bimetallic cooperative O-O bond formation in water oxidation.

Reference:

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