# MS14-2-6 MOF Catalysts for Energy Applications: Incorporation of Transition Metals at Atomic Levels #MS14-2-6

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### Abstract

With the emergency call for carbon neutrality, development of new technologies to produce renewable and clean energy are attracting increasing attention recent years. Hydrogen energy is the most promising one due to that the consumption of hydrogen only produces water. With fuel cell hydrogen can be safely translated to electricity under mild conditions. However, the storage and transmission of hydrogen is still challenging. Ammonia borane as a promising hydrogen storage material can release a high amount of hydrogen with noble metals like Pt, Ru, Rh and Au as catalysts. Besides, in fuel cell devices, platinum group materials are the predominant class of materials that are used as the key component to catalyse the oxygen reduction reaction (ORR). However, the scarcity, high cost, and low efficiency of these noble metal catalysts prevent the widespread implementation of hydrogen as an affordable clean energy.

The low cost yet high tunability of metal-organic frameworks (MOFs) provide a unique platform for tailoring their characteristic properties as new catalysts. I will present stable MOFs with transition metal ions incorporated at atomic level as efficient catalysts. For example, we have developed a series of novel multivariate metal-organic frameworks (MTV-MOFs), MTV-MIL-100, through a solvent-assisted approach[1]. Two Co caions are anchored in each tri-nuclear cluster with ordered atomic arrangements with one Ti cation. These ordered and multivariate metal clusters offer an opportunity to enhance and fine-tune the electronic structures of the crystalline materials. Moreover, mass transport is improved by taking advantage of the high porosity of the MOF structure. Combining these key advantages, MTV-MIL-100(Ti,Co) exhibits a high photoactivity in the photocatalytic hydrolysis of ammonia borane. Moreover, we develop MOF catalysts by combining Zr-chains to promote high chemical stability and metalloporphyrin ligands to introduce transition metal ions as redox active-sites[2]. In addition, we tailor the immobilization and packing of the single redox active atoms at a density that is ideal for the reaction kinetics of ORR. The obtained MOF catalyst, PCN-226, thereby shows high ORR activity. We further demonstrate PCN-226 as a promising electrode material for practical applications in rechargeable Zn-air batteries. These examples represent two different strategies to design and incorporate transition metals in provus materials at an atomic level, which could further accelerate the development in searching for efficient catalysts.

#### References

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