【无机化学论坛】**Molecular Catalysis and Photocatalysis for Water Splitting and CO2 Reduction**

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时间：2019年9月25日（周三） 下午14:00—15:30

地点：北京大学化学学院A区717报告厅.

**报告摘要：**

**Molecular Catalysis and Photocatalysis for Water Splitting and CO2 Reduction**

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Over the past decade, our group has focused on the molecular systems relevant to photosynthetic molecular devices. Our targets involve the studies on (i) water oxidation catalysis in order to uptake protons and electrons required for fuels generation, (ii) catalytic water or CO2 reduction into sustainable fuels (*i.e.*, H2, CO, etc.), (iii) artificial light-harvesting systems towards the effective charge separation and/or migration, and so on. In order to develop the more desirable/efficient systems in promoting all relevant processes, substantial efforts have been devoted to more carefully study the reaction kinetics and equilibria in solution that are relevant to each topic. Various techniques have been adopted to better understand the mechanistic aspects relevant to all of our systems. Some of the reaction steps of interest are not observable by any experimental techniques, and must be discussed on the basis of our DFT results, which also greatly helped us understand the mechanism of reactions. Importantly, one of our findings is that, in any catalysis, the reactivity of metal(s) can be rationally tuned by use of redox active ligands that are more or less hybridized with metal(s) in their orbitals. Such issues are often involved in our discussion. One of our interests has concentrated on the molecular Pt-catalyzed hydrogen evolution reactions and their application in fabricating photosensitizer-catalyst hybrid molecular devices [1-5]. Our recent kinetic and electrochemical studies evidence the formation of a hydridodiplatinum(II,III) intermediate when H2 evolution is catalyzed by a simple mononuclear Pt(bpy)Cl2 derivative, which is also rationalized by our DFT results. Our studies have also provided new aspects on photo-induced multi-charge separation [6], near-infrared-driven water reduction [7], water oxidation catalysis by monocobalt polymolybdate [8], Ru(terpy)(bpy)(H2O) [9], and cobalt porphyrin derivatives [10-12]. Non-precious metal water reduction catalysis using Ni and Co [13-16], and cobalt porphyrin CO2 reduction catalysis in fully aqueous media [17] have also been focused in our recent studies. Moreover, our recent studies further include photoelectrochemical cells for the overall water splitting based on two mesoporous TiO2 films at both the photoanode and the ‘*dark* *cathode’* tethered to a Pt porphyrin water reduction catalyst [18].

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