报告题目：Theoretical Studies on Water Oxidation Catalysts - from Solvent to interfaces
报告时间：2019-07-24 15：00 pm
报告地点：实验三楼 102 会议室
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Water oxidation generates protons and electrons which are elemental components for the generation of the fuel, such as H_2 and CH_3OH. Over the last decade plenty of catalysts were synthesized to accelerate this reaction, however the ways to design efficient and long lived catalysts are still unknown. Understanding the details of the mechanism can help to design a better catalyst with high catalytic performance. Therefore, I applied density functional theory (DFT) to study the rate limiting step in implicit solvent, the empirical valence bond (EVB) method to get insight into the solvent and surface effects, molecular dynamics (MD) and potential of mean force (PMF) methods to perform simulations for large systems at long time-scales. By using these computational techniques, several key properties of the water oxidation catalyzed by Ru-based complexes, such as solvent and surface effects, hydrophobicity, and oxide relay have been investigated in detail. These studies can shed light on the design of molecular water oxidation catalysts with high catalytic activity and will help the development of artificial photosysnthesis devices.