

Internal Webinar

Facile Water Oxidation by Dinuclear Mixed-Valent $\text{Co}^{\text{III}}/\text{Co}^{\text{II}}$ Complexes: Role of Coordinated Water

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Rational design of a catalyst using earth abundant transition metal that can facilitate the smooth O–O bond formation is crucial in developing efficient water oxidation catalysts. We have chosen dinuclear mixed-valent $\text{Co}^{\text{III}}\text{Co}^{\text{II}}$ complexes of the general formula $[\text{Co}^{\text{III}}\text{Co}^{\text{II}}(\text{LH}_2)_2(\text{X})(\text{H}_2\text{O})]$ ($\text{X} = \text{OAc}$ or Cl) that bear a coordinated water molecule in the primary coordination sphere. We anticipated that the water molecule in the primary sphere can take part in proton coupled electron transfer (PCET) mechanism which can accelerate the facile formation of the O–O bond under strong alkaline condition (1M NaOH). To understand the role of the coordinated water we have generated an analogous complex, $[\text{Co}^{\text{III}}\text{Co}^{\text{II}}(\text{LH}_2)_2(o\text{-vanillin})]$ ($o\text{-vanillin} = 2\text{-hydroxy-3-methoxybenzaldehyde}$), without the coordinated water. Interestingly, we have found out that the water coordinated complexes show better oxygen evolution reaction (OER) activity and stability.

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