First-Principles Understanding and Design of Metal Oxides for Solar Hydrogen Production via Water Splitting

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Renewable sources of energy are increasingly needed and solar production of hydrogen fuel from water offers significant potential to contribute to these needs if new photocatalyst materials and/or more efficient photocatalytic systems can be identified for visible-light-driven water photoelectrolysis. Transition metal oxides are considered as promising candidate as they are earth abundant, eco-friendly, and stable in aqueous solution. Particularly, Bismuth Vanadate ($BiVO_4$) has attracted much attention, but pristine $BiVO_4$ exhibits poor electron-hole separation and sluggish water-oxidation kinetics. Significant research efforts have been made to enhance the performance of $BiVO_4$. However, the design and successful realization of commercially viable $BiVO_4$-based photoanodes are still rather elusive. This talk will highlight the strong effects of crystal phase and doping on the photocatalytic activity of $BiVO_4$ that have been found from combined first-principles and experimental studies. The improved understanding offers important guidance for the rational design of metal oxide-based photocatalysts.