Optical and Excitonic Properties Investigation of the Visible Light-Driven Photocatalytic $BiVO_4$ Material

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In 1972, Honda and Fujishima first discovered that it was possible to promote the water splitting reaction, i.e., the decomposition of water into oxygen and hydrogen, by using an electrochemical device based on a TiO_2 anode and a platinum counter electrode exposed to ultraviolet (UV) light[1]. Due to the large band-gap of TiO_2, doping or use of ternary oxides for example $BiVO_4$ opens up another domain of research. In that context, different phases of bismuth vanadate ($BiVO_4$), initially known for its ferroelastic and ionic conductivity properties, is now considered as one of the most promising candidates for solar energy-to-hydrogen conversion processes operating in the visible light range[2,3]. An investigation of the optical and excitonic properties of photocatalytic compounds based on both experimental and theoretical approaches is proposed. More specifically, this research work reports for the first time, the local-field, optical anisotropy, and excitonic effects in $BiVO_4$, an active photocatalytic material in the visible range. The analyses are based on electron energy-loss spectroscopy measurements, ground-state density functional theory calculations, including crystal local-field effects, and many-body corrections using the Bethe-Salpeter equation[4]. These results are supported by a comparison with two materials, namely, TiO_2 anatase and rutile, which are well-known to differ in their photocatalytic properties, those being important and negligible, respectively. The analogies found for these two categories of compounds allow the proposal of criteria that appear to be essential for producing an optimal photocatalytic material.

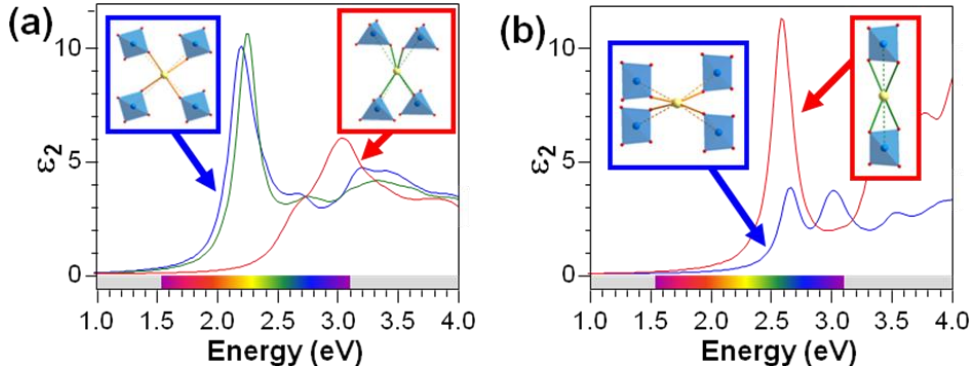

Figure 1 Calculated imaginary part of the dielectric function of monoclinic (a), and tetragonal (b) $BiVO_4$ bulk phases. Calculations are done using Bethe-Salpeter equation in density functional theory formalism.

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