Spectroscopic and first principles characterization of electronic, optical and defect properties of p-type CuBi$_2$O$_4$

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- CuBi$_2$O$_4$, a new p-type semiconductor, is examined with a comprehensive spectroscopic and first principles characterization methodology.

- HSE($\alpha=10.6\%$) properly describes the band gap (1.5eV) and electronic properties of AFM CuBi$_2$O$_4$. Limited PEC performance is explained by lack of Cu-d overlapping at CBM and VBM and lack of connectivity between minority e- and majority h+ conduction paths.

- Our results allowed us to understand features in RIXS spectra. Peaks at low and high emission energy are explained by $\langle \Psi|O-p><Bi-p|\Psi\rangle$ and $\langle \Psi|O-p><Cu-d|\Psi\rangle$ PDOS overlapping.

Understanding oxygen and hydrogen defects in modulating the p-type CuBi$_2$O$_4$ optoelectronic properties

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- We use DFT to compute formation energies and transition levels for hydrogen impurities and oxygen vacancies. Our DFT result show that these defects behave as donors impurities and are harmful for the p-type performance of CuBi$_2$O$_4$. This is contrary to the common situation in n-type semiconductors, where donor impurities are beneficial.

- Experimental Raman peaks display shifts with increasing presence of defects. We use DFT to simulate Raman and compute eigenvectors. High frequency modes have larger contribution of oxygen displacements and are therefore more affected by defects.

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