

## Supporting Information

### First-Principle Investigations of Structural, Electronic, Magnetic and Optical Properties of Bulk BiVO<sub>3</sub>

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**S1:** The computed exchange interactions  $j_i$  are showed in Table below.

**Table:** Values of Spin Exchange Parameters (in meV) of BiVO<sub>3</sub>, determined from GGA+U calculations. The bond length is showed in Fig. 1.

Bond length	V <sub>1</sub> -V <sub>2</sub>	V <sub>1</sub> -V <sub>3</sub>	V <sub>2</sub> -V <sub>4</sub>	V <sub>3</sub> -V <sub>4</sub>
$j_i$	13.45	-6.85	-4.76	8.96

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