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Origins of superior symmetrical doping ability of monoclinic BiVO4 YANFA YAN, WAN-JIAN YIN, SU-HUAI WEI, MOWAFAK AL-JASSIM, JOHN TURNER, National Renewable Energy Laboratory — Application of semiconductors for functional devices depends critically on their dopability. However, there are strong doping bottlenecks for wide-band-gap semiconductors – symmetrical doping is usually difficult, which severely restrict their potential applications. Here, we report superior symmetrical doping properties, i.e., n-type and p-type, of monoclinic $BiVO_4$ by first-principles density-functional theory calculation. Our results reveal that without external doping, $BiVO_4$ with moderate n-type and p-type conductivities can be obtained. However, doping of Sr, Ca, Na, and K atoms under oxygen-rich growth conditions can lead to outstanding p-type conductivity, whereas doping of Mo and W under oxygen-poor growth conditions can result in excellent n-type conductivity. We find that Bi 6s state is responsible for the good p-type doping and the presence of V 3d state is responsible for the good n-type doping. Furthermore, the Bi $6s$ and V $3d$ states are also responsible for producing very dispersive valence and conduction band edges, leading to small electron and hole effective masses. The superior symmetrical doping properties and high carrier mobility make $BiVO_4$ a promising candidate for electronic and optoelectronic device applications.

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