Electronic structure of $BiFeO_3$ in different crystal phases

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Multiferroic $BiFeO_3$ under normal conditions crystallizes in the rhombohedral *R3c* space group. However doping can change its crystal structure to e.g. $Pn2_1a$ (with Gd [1]), *Pnma* (with Gd [1], Y [2]) or *Cm* (with Ga [3]). We present the electronic structure calculations of undoped $BiFeO_3$ in these structures within DFT+U approach. Our structural calculations are in good agreement with previous calculations [4]. Our results show that $BiFeO_3$ favors G-AFM ordering for *R3c*, $Pn2_1a$, *Pnma* structures and C-AFM ordering for *Cm* phase. In all structures $BiFeO_3$ is a semiconductor with the band gap: 2.26 eV (*R3c*), 1.91 eV (*Pnma*), 1.99 eV ($Pn2_1a$), 2.09 eV (*Cm*).

References:

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