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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