Evaluation of Electronic Properties for Crystalline Structures of Ferric Borate Oxides

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Electronic properties for experimentally measured crystalline structures could be very well evaluated by high–level computations. In this respect, ab initio density functional theory (DFT) approaches are powerful tools to characterize the matters in solid phases. [1]. From pure to impure crystals, significant changes are usually arisen in crystalline characters during atomic substitutions in the structural building blocks and geometries, which could be better investigated by computations rather than complicated experiments. Both pure and impure rare–earth crystalline compounds have shown significant advantages especially for electrical applications and technologies. Therefore, it is very much important to evaluate the exact geometries and corresponding properties for such compounds prepared for specific applications. Within this work, crystalline structures and electronic properties for different architectures of ferric borate oxides (FeBO3) [2] have been investigated through experimental measurements and high–level computations as a double–confirmed evaluation. In addition to pure FeBO3, samarium (Sm) rare–earth atom has been substituted in the crystalline structure to build $Sm_aFe_bB_cO_d$ impure crystals. Interestingly, both experiments and computations indicated that the investigated crystals are semiconductors with the capability of applications in electrical technologies. In the experimental section, X–ray absorption near–edge spectroscopy (XANES) [3] has been mainly used to collect data to determine the structural and electronic properties for different samples of $Sm_aFe_bB_cO_d$. In the computational section, high–level DFT computations employing exchange–correlation functionals have been used to evaluate atomic– and molecular–scales configurations of crystalline structures and electronic properties for the investigated SmaFebBcOd compounds. Both experiments and computations have been used to significantly characterize a, b, c, and d atomic portions to determine real structures of Sm–substituted FeBO3 crystals.

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