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**Influence of size effect and electron correlation to the energy band gap of $CuFeO_2$ and $AgFeO_2$** KHUONG ONG, KEWU BAI, Institute of High Performance Computing, Singapore, PETER BLAHA, Inst.f. Materials Chemistry, TU Vienna, PING WU, Institute of High Performance Computing, Singapore — We have calculated the electronic structure of delafossite type oxides $CuFeO_2$ and $AgFeO_2$ using the Full Potential Linearlized Augmented Plane Wave (FP-LAPW) method within Perdew-Burke-Ernzerhof Generalized-Gradient Approximation (PBE-GGA). A metallic state instead of true insulating state is obtained for $CuFeO_2$ and $AgFeO_2$. The insulating state is reproduced when electron correlations have been taken into account. An effective Hubbard parameter for Fe, $U_{eff}$=7.86eV, has been derived based on an ab initio constraint calculation. This value is an over estimation for the optical band gaps of $CuFeO_2$ and most probably for $AgFeO_2$ as well. One reasonable $U_{eff}$ has been derived by comparing between computational and experimental X-Ray emission spectra. The energy band gap of $CuFeO_2$ and $AgFeO_2$ within the PBE-GGA+U is found as charge transfer gap. Theoretical optical band gaps $\Delta_0$=1.30eV, $\Delta_1$=2.06eV, and $\Delta_2$=3.20eV for $CuFeO_2$ are quite compatible with experimental data. For $AgFeO_2$ an optical band gap $\Delta_0$=1.90eV has been predicted. The size effect is considered as the origin of the increase in optical and energy band gaps of $AgFeO_2$ in comparison with $CuFeO_2$.

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