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Study of the electronic and magnetic properties of $A_2Ti_2O_7$ (A=Er, Tb)

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Abstract

The geometrical frustration in the magnetic pyrochlore oxides causes interesting properties at low temperatures in these materials. Therefore, we studied two challenging materials, $Er_2Ti_2O_7$ and $Tb_2Ti_2O_7$, using an ab initio method, based on Density Functional Theory (DFT). To take into account the f electrons coulomb interactions correctly, we employed DFT+U, a Hubbard method correction. As spin-orbit coupling (SOC) is very effective in these materials, we added SOC to the DFT+U calculations (DFT+U+SOC). Using DFT+U+SOC, we examined the effect of non-collinear magnetism. The DFT+U+SOC calculations give rise to the magnetic moments $8.2 \mu_B$ and $7.1 \mu_B$ for $Er_2Ti_2O_7$ and $Tb_2Ti_2O_7$, respectively. These values deviate from the experimental results. The reason is that the DFT calculations are trapped in the local minima, indicating that we need more sophisticated methods to find the global minimum in our electronic structure calculations. Although we need structural optimization to find better magnetic moment values, unfortunately it is possible to reach incorrect structural optimization if the electronic structural optimization for finding global minima is not performed correctly.

Keywords: magnetic pyrochlore oxides, geometric frustration, density functional theory, collinear magnetization

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