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Prediction of a Low Band Gap Oxide Ferroelectric[1] DAVID SINGH, ORNL, BO XU, National University of Singapore, VALENTINO R. COOPER, ORNL, YUAN PING FENG, National University of Singapore — We report a first principles study of $Bi_6Ti_4O_{17}$ which is an alternate stacking of ferroelectric $Bi_4Ti_3O_{12}$ (BiT). We the standard PBE GGA functional for the structure and polarization and a recently developed functional that yields accurate band gaps for the electronic structure. We find that this compound is ferroelectric although with a reduced polarization relative to BiT. Importantly, calculations of the electronic structure yield a band gap of approximately 1.4 eV. Therefore, we predict that this stacking is a low band gap oxide ferroelectric.

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