Direct band gaps in multiferroic h-LuFeO₃

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Abstract :

We measured the optical properties of epitaxial thin films of the metastable hexagonal polymorph of LuFeO3 by absorption spectroscopy, magnetic circular dichroism, and photoconductivity. Comparison with complementary electronic structure calculations reveals a 1.1 eV direct gap involving hybridized Fe $3d_z^2$ + O $2p_z$ to Fe *d* excitations at the Γ and A points, with a higher energy direct gap at 2.0 eV. Both charge gaps nicely overlap the solar spectrum.