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The electronic structure of FeTiO₃

Magnetic transition metal oxide structures with ABO₃ type stoichiometry offer a wide range of technologically important properties including ferroelectricity, ferromagnetism and colossal magnetoresistance, piezoelectricity, multiferroicity, and metal–insulator transitions. In the case of FeTiO₃ its magnetic behaviour may be switched through use of a magnetic field which influences whether there is, or is not, some measurable magnetisation. This in part may be due to the possibility that FeTiO₃ is unstable to energy-lowering structural distortions through cation-cation and cation-anion interaction. A photoemission study is presented that explores these ideas through the experimental and theoretical determination of the valence band structure as well as chemical states of the material after several processing steps. DFT calculations, Wien2k, are used to determine the chemical character of bonding and related to the various types of magnetic phase found in FeTiO₃.

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