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First Principles Calculation of Helical Spin Order in Iron Perovskite SrFeO3 and BaFeO3 ZHI LI, Yukawa Institute for Theoretical Physics, Kyoto University — Motivated by recent discovery of ferromagnetism in cubic perovskite BaFeO3 under small magnetic field, we investigate spin order in BaFeO3 and isostructual SrFeO3 by a first principles calculation using local spin density approximation (LSDA). We find that on-site Coulomb interaction U is necessary for obtaining helical spin order consistent with experiments. SrFeO3 exhibits G-type helical order, while BaFeO3 exhibits the A-type with very small wave vector. The A-type order is stabilized by lattice expansion. Small energy difference between the A-type and ferromagnetic orders explains ferromagnetism under small field. The LSDA+U results are consistent with model calculation where negative charge-transfer energy in these compounds is explicitly taken into account.

Zhi Li
Yukawa Institute for Theoretical Physics, Kyoto University

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