

Abstract Submitted
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Highly accurate calculation of the magnetic properties of FeSe and FeTe using first principles quantum Monte Carlo¹ BRIAN BUSEMEYER, University of Illinois at Urbana-Champaign, MARIO DAGRADA, SANDRO SORELLA, University Pierre et Marie Curie, MICHELE CASULA, SISSA, LUCAS K. WAGNER, University of Illinois at Urbana-Champaign — While the origin of superconductivity in the iron-based materials is still controversial, the proximity of the superconductivity to magnetic order is suggestive that magnetism may be important. We use first principles quantum Monte Carlo (QMC) techniques to obtain an accurate microscopic picture of the effects of magnetic configurations on the electronic structure of FeSe under pressure. The QMC calculations reproduce experimental values for bulk modulus, lattice constants, bandwidth, and lowest energy magnetic ordering. The relative energy of magnetic orderings is rather different from standard density functional theory calculations, which may warrant a reassessment of the role of magnetism in this material. We analyze the correlated wave functions to obtain a microscopic explanation for the spontaneous S4 symmetry-breaking in this material, and contrast these results with the non-superconducting case of FeTe.

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