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2024 APS March Meeting
Monday–Friday, March 4–8, 2024; Minneapolis & Virtual

Session T01: Nematicity, Correlations and Pairing
11:30 AM–1:18 PM, Thursday, March 7, 2024
Room: L100A

Sponsoring Unit: DMP
Chair: Qing-Ping Ding, Ames National Laboratory

Abstract: T01.00005 : Spin and orbital degrees of freedom in FeSe: ab-initio perspective (Part-I)*

12:18 PM–12:30 PM

Abstract

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FeSe is the structurally simplest quasi-two-dimensional iron chalcogenide superconductor. In spite of the structural simplicity, its phase diagram presents exotic phases (superconductivity, spin density wave, nematicity) which are the object of intense study by the condensed matter community. At fundamental level, the description of the orbital and spin degrees of freedom and of their interaction is key to understand the properties of FeSe in its different phases.

We present the calculations of structural, electronic, and magnetic properties of FeSe in the tetragonal phase within density-functional theory at the generalised gradient approximation level. First, we studied how the bandwidth of the d-bands at the Fermi energy are changing by adding simple corrections: Hubbard U, Hund's J and by introducing long-range magnetic orders. We found that introducing either a striped or a staggered dimer antiferromagnetic order brings the bandwidths—which are starkly overestimated at the generalized gradient approximation level—closer to those experimentally observed. Second, for the ferromagnetic, the striped, checkerboard and the staggered dimer antiferromagnetic order, we investigate the change in magnetic formation energy with local magnetic moment of Fe at a pressure up to 6 GPa. The bilinear and biquadratic exchange energies are derived from the Heisenberg model and noncollinear first principles calculations, respectively. We found a non-trivial behaviour of the spin-exchange parameters on the magnetization and we put forward a field-theory model that rationalizes these results in terms of strongly coupled, two-dimensional spin-orbital fluctuations. The implications for the experimentally observed phase diagram are then discussed.

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