Phonon and electron densities in tetragonal and orthorhombic FeSe versus pressure

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The simplest superconductor belonging to the newly discovered iron-based class of superconductors belongs to the binary iron-selenium system. Superconductivity with the transition temperature T_c=8 K has been discovered for a compound being formed close to the FeSe stoichiometry with excess iron. This compound has *P4/nmm* tetragonal structure at room temperature and transforms into *Cmma* orthorhombic phase between 100-80 K. It was found that T_c strongly depends upon applied pressure raising to 36.7 K at 8.9 GPa and subsequently dropping due to the induced phase transition into some hexagonal structure. Therefore, it is important to look upon phonon and electron density of states versus pressure in this unconventional compound to decide what kind of the boson field is responsible for the Cooper pairs formation. We have already found that there is no electron spin polarization within the unit cell [1].

Calculations are performed for the stoichiometric compound within the density functional theory (DFT) implemented in VASP code [2]. Local density approximation (LDA) is used as better suited for the refinement of the crystal structure. A harmonic approximation is used to study lattice dynamics of the system [3].

Results of the calculations are to be discussed in detail. Preliminary calculations show that the iron magnetic moment is zero in the ground state of both phases. It has been found that transition from tetragonal to the orthorhombic phase is driven by decrease of the zero-point motion energy, while going to the ”softer” orthorhombic phase.

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