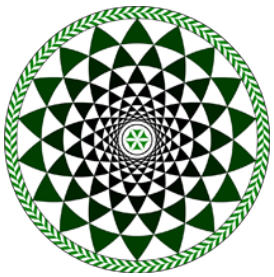

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Structural phase transition in KFe_2As_2 from ab initio calculations

Thursday, 6 July 2017 13:00 (20 minutes)

KFe_2As_2 belonging to the most investigated family of iron-based superconductors, AFe_2As_2 (A = alkali metal or alkali earth metal) is the first self-doped iron pnictide compound that does not need chemical substitutions or imposing of pressure to superconduct. However, the superconducting transition temperature, 3.8 K, is rather low [1]. It rises with partial substitution of Sr or Ba atoms for K atoms to 37 K [1] or 38 K [2], respectively. In contrast to other AFe_2As_2 (A=Ca,Ba,Eu,Sr) compounds that exhibit a structural phase transition from a high-temperature tetragonal to a low-temperature orthorhombic phase, followed by an antiferromagnetic spin density-wave transition the crystal structure of KFe_2As_2 remains tetragonal down to lowest temperatures. Also, no magnetic order develops in that material. Under pressure, the tetragonal phase transforms to the collapsed tetragonal (cT) phase with the same symmetry but with strong and extremely anisotropic changes of the lattice parameters [3]. The cT phase of KFe_2As_2 is superconducting with T_c=12 K.

To obtain a deeper insight in the mechanism of the phase transition in KFe_2As_2 the structural, electronic and dynamical (phonon) properties of the crystal under pressure have been studied using the first-principles calculations. The crystal structure optimization under various pressures were performed using the projector augmented-wave formalism of the Kohn-Sham density functional theory (DFT) within the generalized gradient approximation (GGA) approach in PAW-PBE form, implemented in the Vienna ab initio simulation package (VASP). It has been shown that the source of this transformation is the formation of the As-As bonds between initially non-bonded As-As atoms caused by the overlap of $4p_z$ orbitals being a result of imposed pressure.

References

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Primary author: Dr STERNIK, Małgorzata (Institute of Nuclear Physics, Polish Academy of Sciences)

Co-authors: Dr PTOK, Andrzej (Institute of Nuclear Physics, Polish Academy of Sciences); Prof. PIEKARZ, Przemysław (Institute of Nuclear Physics, Polish Academy of Sciences)

Presenter: Dr STERNIK, Małgorzata (Institute of Nuclear Physics, Polish Academy of Sciences)

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