Nanoobjects microscopy

The surface influence on the orbital and the spin states of iron chalcogenides nanoparticles.

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In the iron-containing superconducting chalcogenides, the major building block is a layer of edge shared tetrahedrons FeX_4 (X = S, Se, Te) with $3d^6$ divalent iron ion in the center. The closeness of Hund and crystal field energy allows easy switching between three different spin state of iron ions which in turns accompanies by the orbital re-populations. Therefore iron chalcogenides family shows large variety of physical properties which varies from magnetic insulators with Fe in the high spin state (S=2) to superconductors with Fe in low spin state (S-0). Furthermore, tetrahedron distortions (e.g. pressure application) can cardinally change spin state and conductive and magnetic properties. In our papers [1-4] we show that B_{1g}(Fe) phonon mode can be a marker of the iron spin state. In our report using modified crystal field approach we study the variation of the iron ion adiabatic potential under influence of different types the [FeX_4] tetrahedron distortions which are expected at the surface of the nanoparticles. We show that in the proximity to the spin state instability the adiabatic potential has asymmetric form depending on the sign of distortions that could lead to the drastic difference of physical properties between bulk and nanoparticles of these compounds.

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2. *Пашкевич Ю.Г., Шевцова Т.Н., Гусев А.А., Гнездилов В.П., Lemmens P.* Спиновое состояние железа - управляющий параметр железосодержащих ВТСП: зависимость энергии основного состояния, энергий фононов и позиций атомов от спинового состояния иона железа в FeTe // ФНТ. – 2012. – **38**. – С. 1135-1140.

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