Superconductivity and JT polarons in titanates

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High temperature superconductors (HTSC) cuprates and titanates have a number of similarities at the fundamental level. Both structures can be described in terms of perovskite−type lattices. Recently it was discovered that both type of crystals show the presence of Jahn−Teller (JT) polarons and their strong coupling to lattice vibrations. It is also known that both materials may exhibit the superconductivity phenomenon. In the present work we use a quantum−chemical method developed for crystal studies. We focus on the following two features: (i) superconductivity in the La−doped $SrTiO_3$ crystal, and (ii) JT polarons in the $BaTiO_3$ crystal. In the case of $SrTiO_3$ crystal our study [1] shows the occurrence of free electrons in the conduction band of the crystal and explains a number of the experimental results obtained for the superconducting La−doped $SrTiO_3$ existing under 14K. The free electrons are found to be situated on the Ti−O planes similar to the case of free electrons situated on Cu−O planes in the HTSC cuprates. The lattice might disperse the wave functions of the free electrons. However, due to the periodicity the dispersed waves in the superconducting state will be interfering constructively. Thus the gaps between the maximums should match exactly the distance between the superconducting planes in the $SrTiO_3$ crystal allowing the electrons to travel without any resistance.Studies of the JT polarons in the $BaTiO_3$ crystal [2] have showed possibility of occurrence of JT polarons in a pure $BaTiO_3$ lattice explaining a number of experimental observations and matching some important results obtained independently by the polaron theory for the $BaTiO_3$ crystal and the HTSC cuprates. In particular, the calculated JT polaron binding energy, −0.87 eV, practically matches the corresponding value, −0.842 eV, obtained by the polaron theory using the so−called Frohlich electron−phonon interaction [3].Our studies imply that the superconductivity and the localized JT polarons in the HTSC cuprates and titanates could be a consequence of another fundamental, still undiscovered phenomenon present in these crystals. Depending on conditions may occur one of the two competing phenomena, either the superconductivity or the JT charge− and spin−ordered phases.

1. P. Sanchez and A. Stashans, Phil. Mag. B, 81, 1963 (2001).
2. H. Pinto and A. Stashans, Phys. Rev. B, submitted (2001).
3. A. S. Alexandrov and A. M. Bratkovsky, J. Phys.: Condens. Matter 11, L531 (1999).