

Microscopic Study of the Role of Structural Distortion in Oxypnictide Superconductors: A Two Band Approach

S S JENA¹, S K AGARWALLA¹ and G C ROUT^{2*}

¹Dept of Applied physics and Ballistics, F.M. University, Balasore 756019, Odisha, India, ²Physics Enclave, Plot No. - 664/4825, Lane-4A, Shree Vihar, Chandrasekharpur, PO- Patia, Bhubaneswar- 751031, Odisha, India, Mob: 09937981694.

*Corresponding author: Email Id: gcr@iopb.res.in,

¹Email Id: sushree@iopb.res.in, Mob: 08895084073.

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Abstract. The doped oxypnictides of type 1111 exhibit verities of lattice distortions. We propose here a tight-binding two band model to explain the temperature dependent lattice strain in this system. The two band tight-binding model consists of nearest neighbor and next-nearest-neighbor electron hoppings. The lattice distortion arising due to lattice strain is proposed to be investigated by incorporating JT type distortion in which the d_{xz} band is raised by Jahn-Teller (JT) energy, Ge and the d_{yz} band is suppressed by JT energy, $-Ge$, so that there exists a JT gap of energy, $2Ge$. This provides a strong interplay between the lattice energy and the electronic energy to stabilize the system. The lattice strain and hence the JT energy are calculated by using Zubarev's Green's function technique. Finally the lattice strain is computed self-consistently. The temperature dependent lattice strain exhibits a mean-field behavior exhibiting a tailing nature near the lattice distortion temperature. This indicates that the lattice strain is not robust but gradual near the transition temperature. The temperature dependent lattice strain is investigated by varying the physical parameters like JT coupling, elastic constant, different hopping integrals and chemical potential. The results are discussed in the text.

Keywords: Iron-based superconductors, Jahn-Teller effect.

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