Effective five band analysis on T_c vs. lattice structure correlation in iron pnictides

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The discovery of superconductivity in the iron pnictides [1] and its T_c up to 55K [2] has given great impact to the field of condensed matter physics. From the early stage, much attention has been paid to the correlation between T_c and the lattice structure [3]. In the present study, we focus on the condition for optimizing superconductivity in the iron pnictides, varying hypothetically the lattice structure. Studying the band structure of the hypothetical lattice structure of LaFeAsO, the hole Fermi surface multiplicity is found to be maximized around the Fe-As-Fe bond angle regime where the arsenic atoms form a regular tetrahedron. Superconductivity is optimized within this three hole Fermi surface regime, thereby providing a natural explanation as to why T_c is optimized around the regular tetrahedron angle. Combining also the effect of varying the Fe-As bond length, we provide a guiding principle for obtaining high T_c.

[1]Y.Kamihara *et al.*, J. Am. Chem. Soc. **130**, 3296 (2008).
[2]Z-A Ren *et al.*, Chinese Phys. Lett. **25**, 2215 (2008).
[3]C.H. Lee *et al.*, J. Phys. Soc. Jpn. **77**, 083704 (2008).