Effective five band analysis on the lattice structure effect in iron pnictides

HIDETOMO USUI, KAZUHIKO KUROKI, The University of Electro-Communications — The discovery of superconductivity in the iron pnictides\cite{1} and its $T_c$ up to 55K\cite{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\cite{3}. In the present study, we focus on the condition for optimizing superconductivity in the iron pnictides, varying hypothetically the lattice structure of LaFeAsO. 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 the varying the Fe-As bond length, we provide a guiding principle for obtaining high $T_c$. \cite{1}Y.Kamihara et al., J. Am. Chem. Soc. 130, 3296 (2008). \cite{2}Z-A Ren et al., Chinese Phys. Lett. 25, 2215 (2008). \cite{3}C.H. Lee et al., J. Phys. Soc. Jpn. 77, 083704 (2008).

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