Electronic states and material dependences of Fe-based superconductors MICHIYASU MORI, IMR, Tohoku Univ., TAKAMI TOHYAMA, Kyoto Univ., NAVID AFZAL SHOOSHTARY, SADAMICHI MAEKAWA, Tohoku Univ. — In this study, we will discuss the electronic states of Fe- based superconductors and its material dependences, in particular, by taking account of the bond angle dependences. First, we calculate the crystal field splitting (Δ) of Fe 3d orbital coordinated by four As's. Next, the hopping integrals (t) are estimated by using the Slater and Koster fs method. Note that these parameters, t and Δ change with α. Finally, we can obtain the dispersion relation as a function of α. It is found that the spectral weights near the Fermi energy are dominated by yz, zx and x2-y2 orbitals. The yz and zx orbitals are higher in energy around the regular tetragonal geometry, in which α is almost 109°. On the other hand, those two orbitals become lower in energy for the larger value of α. Such an orbital crossing is crucial for the electronic states. The ground state phase diagram is obtained by the Hartree-Fock calculation of multi-band Hubbard model.

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