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Role of bonding angle on superconductivity in iron pnictide: Comparative electronic structure study on LiFeAs and $Sr_4V_2O_6Fe_2As_2$
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— The special relation between As-Fe-As bonding angle and superconductivity is the most remarkable universal feature in iron-based supercondutor. The maximum Tc can be achieved only with the certain bonding angle, the optimal angle that makes $FeAs_4$ tetrahedron regular. Despite its importance, a hinge behind the relationship between bonding angle and Tc is unclear and less considered so far. In this presentation, we present the comparative electronic structure study on two representative systems, LiFeAs and $Sr_4V_2O_6Fe_2As_2$. LiFeAs has small bonding angle with relatively lower Tc at 18 K and $Sr_4V_2O_6Fe_2As_2$ shows higher Tc at 37 K and its bonding angle is close to the optimal value. Using ARPES, the band dispersion including kz dependence and its orbital characters are explored. Detailed analysis reveals only $Sr_4V_2O_6Fe_2As_2$ electronic structure has orbital mixed nature and relatively strong Fermi surface nesting instability. Both feature indicate strong inter-orbital coupling and its possible role to the superconductivity, which can be the hinge between bonding angle and Tc.

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