Electronic Structure of $A_yFe_{2-x}Se_2$ from First Principles$^1$ CHAO CAO, JIANHUI DAI, Hangzhou Normal University

— The newly discovered $A_yFe_{2-x}Se_2$ iron-selenide material family was studied in a series of first-principles simulations. The electronic structure and magnetic properties of possible vacancy-superstructure phases $A_2Fe_3Se_4$ and $A_2Fe_4Se_5$, as well as the possible parental phase of superconductivity $AFe_2Se_2$ were examined. It was discovered that $AFe_2Se_2$ ground state is a SDW-AFM metal without hole Fermi-surface, thus FS-nesting is absent and its magnetism is very likely to be local moment; $A_2Fe_3Se_4$ is a Mott insulator with SDW-AFM magnetism; $A_2Fe_4Se_5$ shows block-spin AFM ground state with $400\sim 600$ meV band gap. Under high pressure, the $A_2Fe_4Se_5$ phase exhibits rich and exotic physical properties.

[1] Chao Cao and Jianhui Dai, Block Spin Ground State and Three-Dimensionality of (K,Tl)$_y$Fe$_{1.5}$Se$_2$, Phys. Rev. Lett. 107, 056401 (2011)

$^1$NSFC and NSF Zhejiang Province

Chao Cao
Hangzhou Normal University

Date submitted: 01 Dec 2011

Electronic form version 1.4