Abstract Submitted
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Electronic Structure of $A_yFe_{2-x}Se2$ from First Principles[1] CHAO CAO, JIANHUI DAI, Hangzhou Normal University — The newly discovered $A_yFe_{2-x}Se2$ 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 AFe2Se2 were examined. It was discovered that AFe2Se2 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∼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 $(K,Tl)_yFe_{1.6}Se_2$, *Phys. Rev. Lett.* **107**, 056401 (2011)
[2] Chao Cao and Jianhui Dai, Electronic structure and Mott localization of iron-deficient $TlFe_{1.5}Se_2$ with superstructures, *Phys. Rev. B* **83**, 193104 (2011)
[3] Chao Cao and Jianhui Dai, Electronic Structure of KFe_2Se_2 from First-Principles Calculations, *Chin. Phys. Lett.* **28**, 057402 (2011)

[1]NSFC and NSF Zhejiang Province

Chao Cao
Hangzhou Normal University

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