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Density Functional Study of $ThCr_2Si_2$-type Ternary Iron Chalcogenides: $TlFe_2X_2$ (X = S, Se, Te)[1] LIJUN ZHANG, DAVID SINGH, Oak Ridge National Laboratory — We report density functional calculations of electronic structure, Fermi surface, and magnetism for ternary iron chalcogenides $TlFe_2X_2$ (X = S, Se, Te). $TlFe_2S_2$ and $TlFe_2Se_2$ were experimentally synthesized with the $ThCr_2Si_2$-structure, which consist of alternated Fe-X and electron-doping Tl layers, very similar to ternary $BaFe_2As_2$ system. As in all the Fe-based superconductors, the electronic structure near the Fermi level is dominated by Fe 3d states, with a pseudogap. Tl occurs with valence Tl^+, and thus provides heavy electron-doping with 0.5 additional carrier per Fe relative to Fe-X layers. This pushes the Fermi level to the upper edge of the pseudogap and results in disappearance of hole cylinders of Fermi surface at zone center. As expected, the spin density wave instability is completely suppressed and the checkboard antiferromagnetism becomes the favored magnetic order. This over-doped system may be helpful in elucidating the magnetic order, superconducting mechanism, and spin pseudogap behavior in Fe-based materials. Tl deficiency is predicted to reinstate the part of hole Fermi surface and again induce spin fluctuations corresponding to the spin density wave, which are essential for pairing states in Fe- based superconductors.

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