ELECTRONIC STRUCTURE AND MAGNETISM OF Fe-BASED SUPERCONDUCTORS

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S u m m a r y

Ab initio calculations of the electronic structures are carried out for the novel $FeSe_{1-x}Te_x$ superconductors to explain the experimentally found anomalous magnetic properties in the normal state. The calculations have shown that $FeSe_{1-x}Te_x$ systems are close to a magnetic instability with dominating enhanced spin paramagnetism. The magnetic susceptibility is found to increase gradually with the Te content. The temperature dependences of the magnetic susceptibility χ and its anisotropy $\Delta\chi = \chi_{\parallel} - \chi_{\perp}$ are investigated for FeSe, and a growth of the susceptibility with the temperature is revealed in the temperature range 4.2–300 K. For FeTe, a substantial increase of χ under pressure is found. The calculated paramagnetic susceptibility exhibits a strong dependence on the unit cell volume V and especially the height of chalcogen species from the Fe plane. The calculations have explained the experimental data on $\chi(T)$ and $\chi(P)$ for FeSe and FeTe, respectively.