

Magnetism, self-doping and incipient Mott Physics in the Fe-intercalated Fe-selenide $\text{LiFeO}_2\text{FeSe}$

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A series of recent experiments has shown that the magnetic order and superconducting critical temperatures of Fe selenides can be tuned by intercalation with foreign atoms, molecular layers, or epitaxial growth. In this work, [1] we employ a combination of density functional theory (DFT) and dynamical mean field theory (DMFT), to show the electronic structure of a very special intercalated selenide, which was reported to be superconducting with a critical temperature (T_c) of 43 K in the fall of 2013. [2] In this compound, with chemical formula $\text{LiFeO}_2\text{FeSe}$, the FeSe layers alternate with LiFeO_2 layers. Together with $\text{Sr}_2\text{VO}_3\text{FeAs}$, [3] this is to date the only example of iron-based superconductor with a magnetic buffer layer. What makes this compound even more special is that the magnetic atom in the buffer layer - Fe(Li) - is also an iron atom, but in a nominal d^5 configuration, while the iron in the chalcogenide planes - Fe(Se) - is in the usual d^6 configuration of Fe-based superconductors.

At a DFT level, both layers contribute states to the Fermi surface, which is therefore more complicated than in usual FeSe superconductors. The ground state is an antiferromagnetic metal, in which Fe(Li) and Fe(Se) have sizable magnetic moments - 3.6 and 2.6 mB respectively - with a strong mutual antiferromagnetic coupling. Including dynamical correlations in DMFT results in a very different behavior for the two Fe atoms: Fe(Se)-derived bands retain a quasi-particle character, with a mass renormalization comparable to that of pure FeSe [4]; on the other hand, since Fe(Li) is close to an orbital-selective Mott transition regime, [5] the relative bands have a strongly incoherent character and are almost completely removed from the Fermi level.

[1] C. Heil et al, Phys. Rev. B (in press).

[2] X.F. Lu et al, Phys. Rev. B 89, 020507R, 2014.

[3] X. Zhu et al., Phys. Rev. B 79, 220512R, (2009).

[4] M. Aichhorn et al., Phys. Rev. B 82, 064504 (2010).

[5] L. de Medici et al., Phys. Rev. Lett. 107, 256401 (2011).