Spin Fluctuation Calculations of Pairing in Ammoniated FeSe

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Introduction

In the recently synthesized Lix(NH2)y(NH3)zFe2Se2 family of iron chalcogenides, a molecular spacer consisting of lithium ions, lithium amide and ammonia separates layers of FeSe. It has been shown that upon variation of the chemical composition of the spacer layer, superconducting transition temperatures can reach T_c ~ 44 K, but the relative importance of the layer separation and effective doping to the T_c enhancement is currently unclear. Using state of the art band structure unfolding techniques, we constructed eight-orbital models from ab-initio density functional theory calculations for these materials. Within an RPA spin-fluctuation approach, we showed that the electron doping enhances the superconducting pairing, which is of s_-symmetry and explain the experimentally observed limit to T_c in the molecular spacer intercalated FeSe class of materials.

Results and Discussion

We first performed density functional theory calculations for Li0.5(NH2)y(NH3)zFe2Se2 for various y and z. These calculations were downfolded onto 10-orbital, 3D tight-binding models, which served as inputs for spin fluctuation calculations of the pairing vertex in the FeSe ammoniated materials. This is a multiorbital generalization of the Berk-Schrieffer approximation for the pairing vertex, varying both doping and layer separation.

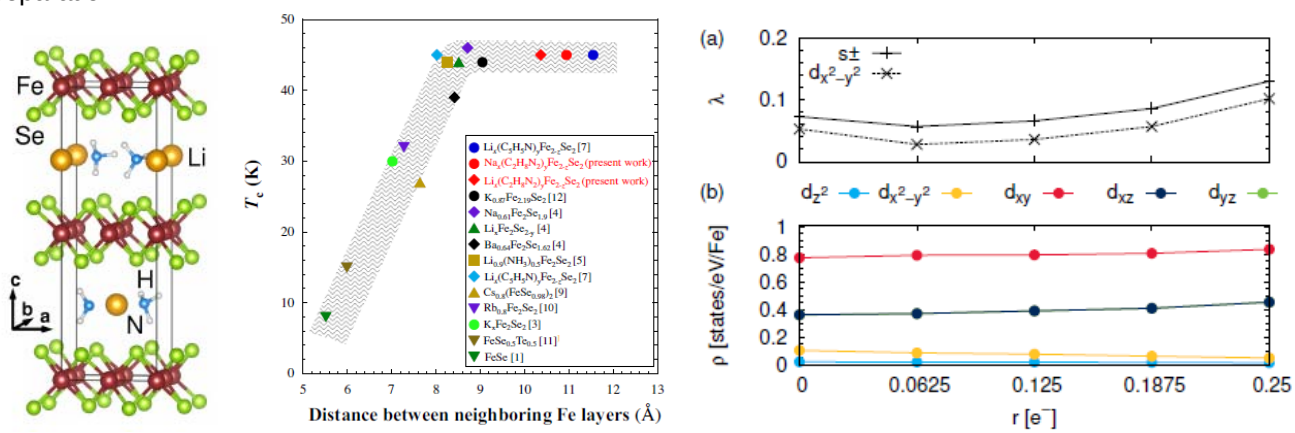

Figure 1 (Left) Structure of Li-ammonia intercalates of FeSe (Middle) Trend of T_c with FeSe interlayer distance [1]. (Right) Trend of the eigenvalues of s_ and dx2-y2 solutions (a) and orbital resolved Fe 3d density of states at the Fermi level (b) with doping.

Conclusions

For the Lix(NH2)y(NH3)zFe2Se2 family of FeSe intercalates, we found that the FeSe layer is moderately electron doped. The electron doping moves the Fermi level towards the edge of the hole-bands, which gives rise to increased superconducting transition temperatures due to an increase in the density of states at the Fermi 5 level. We also showed that recently achieved interlayer distances in FeSe intercalates already produce a two-dimensional Fermi surface, which is optimal for T_c. We concluded that further experimental work should concentrate on the charge doping through the spacer layer.

Acknowledgements

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References

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[2] D. Guterding, P.J. Hirschfeld, and R. Valenti, submitted to Phys. Rev. Lett., arXiv:1410.7565