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Magnetic, structural and superconducting phase diagram in bulk Fe chalcogenides: role of nematic fluctuations and biquadratic exchange[1]

IGOR MAZIN, Naval Research Lab

It has been recently realized that even the bulk FeSe is distinctly unusual, compared to "old" pnictogen-based Fe based superconductors (FeBS), which may be a clue to understanding more exotic FeSe-derivatives. The mystery starts with the FeSe phase diagram: numerous pnictides experience an orthorhombic transition, likely of "spin-nematic" nature, followed by a magnetic transition; external pressure favors superconductivity if the starting phase is magnetic, and suppresses it otherwise, consistent with pressure suppressing spin fluctuations. FeSe, however, experiences an orthorhombic transition with no apparent sign of magnetic ordering, and its Tc raises rapidly with pressure, before switching to the usual, opposite trend. In this talk I will revisit, based on DFT calculations, magnetic interactions in chalcogenides, and show that they, unlike pnictides, demonstrate unusual (and unanticipated) frustration, which suppresses magnetic, but not nematic order, and fully explain the non-monotonic $T_c(P)$. Specifically, after the discovery of FeBS multiple attempts have been made to map the magnetic interactions in these systems (deemed to be crucial for superconductivity) onto a set of short range pairwise exchange interactions, initially in terms of the $J_1 - J_2$ Heisenberg model HM. This approach failed to explain the double-stripe magnetism in FeTe, so the model was extended to include J_3. However, it was soon realized that this HM contradicts both *ab initio* calculations and neutron experiments in the magnetically ordered state of Fe pnictides. Thus the model was augmented to include a nearest neighbor biquadratic exchange K. It was also appreciated that the same interaction is essential for explaining the splitting between antiferromagnetic and orthorhombic phase transition in Fe pnictides. What has not been appreciated though was that (1) the double-stripe order is never a ground state of the HM, independent of the values of $J_{1,2,3}$; it can be stabilized only through K, (2) the HM model has, in addition to usually considered in FeBS phases, a highly competitive novel antiferromagnetic "staggered stripes" phase, which appears to be the ground state in ab initio calculations for FeSe (but not FeTe or for FeSe under pressure). Applying the full $J_{1,2,3} + K$ model to the Fe(Se,Te) system demonstrates unusual frustration, not relevant for As-based FeBS, which can explain the phase diagram of the system, nonmonotonic behavior if Tc under pressure and unexpectedly large orthorhombic "nematic" region in the FeSe phase diagram.

[1]The work performed in collaboration with J. Glasbrenner, H. Jeschke, M. Tomic and R. Valenti.