Electronic structures and magnetic orders of iron- pnictides or chalcogenides

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The first-principles electronic structure calculations play an important role on study of high Tc superconductor iron- pnictides or chalcogenides. Iron-pnictides were first predicted by the theoretical calculations to be antiferromagnetic semimetals [1]. Based on the calculations, Arsenic-bridged antiferromagnetic superexchange interaction was proposed [2]. The bi-collinear antiferromagnetic order was then predicted for iron-chalcogenide α-FeTe [3]. Recently, the parent compounds of superconductors iron-chalcogenides $K_yFe_{2-x}Se_2$ with ordered Fe vacancies were further shown to be antiferromagnetic semiconductors [4], in which the superconductivity emerges upon electron or hole doping, especially, the superconductivity and antiferromagnetic long-range order coexist. It was then proposed that the superconductivity is driven by mediating coherent spin wave excitations in these materials $K_yFe_{2-x}Se_2$ [5].

[1]Phys. Rev. B **78**, 033111 (2008)
[2]Phys. Rev. B **78**, 224517 (2008)
[3]Phys. Rev. Lett. **102**, 177003 (2009)
[4]Phys. Rev. Lett. **106**, 087005 (2011); arXiv:1102.2215
[5]arXiv:1102.4575

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