Electronic structures and magnetic properties ofiron- 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. Based on the calculations, Arsenic-bridged antiferromagnetic superexchange interaction was proposed. The bi-collinear antiferromagnetic order was then predicted for iron-chalcogenide alpha-FeTe. Recently, the parent compounds of superconductors iron-chalcogenides KyFe2-xSe with ordered Fe vacancies were further shown to be antiferromagnetic semiconductors, in which the superconductivity emerges upon electron or hole doping, especially, the superconductivity and antiferromagnetic long-range order may coexist

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