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First principles study of magnetic interactions and electronic structure in iron chalcogenide superconductors MYUNG JOON HAN, SERGEY Y. SAVRASOV, University of California, Davis — By using first-principles density functional theory combined with linear response theory we investigate the magnetic interaction of the Fe chalcogenide high T_C superconductors, $FeSe_{1-x}Te_x$. The calculated exchange interactions are found to be different from those in pnictides, which suggests possibly different superconducting properties. The nearest neighbor antiferromagnetic coupling (J_{1a}) is much stronger than the nearest neighbor ferromagnetic (J_{1b}) and the next nearest neighbor coupling (J_2). The J_{1a} and J_2 gradually decreases as x increases while J_{1b} increases and becomes to be stronger than J_2. Total energy calculation results and the electronic structure will be presented and compared to recent experiments.

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