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Density functional study on anisotropic magnetic exchange couplings in iron-based superconductors HYUNGJU OH, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — Iron-based superconductors exhibit many different antiferromagnetically ordered ground states. An understanding of the magnetic exchange couplings and ground-state Hamiltonian in the parent compounds of these materials is important because such an information could be the basis to unveil the mechanism of unconventional superconductivity. By performing first-principles calculations of the electronic and magnetic properties with non-collinear spin configurations, we study the anisotropic magnetic exchange couplings in iron-based superconductors. We obtain magnetic excitations using the anisotropic magnetic exchange couplings, and compare the results with published inelastic neutron scattering data. This work was supported by the NRF of Korea (Grant No. 2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2012-C2-14).

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