Magneto-crystalline anisotropy in Fe pnictides

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Abstract

If spin-orbit coupling is taken into account, LSDA band structure calculations for parent Fe pnictides successfully reproduce the correct magnetic ground state with stripe antiferromagnetic (AFM) order and Fe moments aligned along a, i.e., along AFM Fe chains. They also predict that the out-of-plane (ac) magneto-crystalline anisotropy (MCA) in LaFeAsO and $BaFe_2As_2$ is stronger than the in-plane (ab) one. However, recent polarized inelastic neutron scattering experiment showed the opposite: the gap at zone center is larger for in-plane spin excitations than for out-of-plane ones, which means that it is easier to deviate Fe spins in the ac plane. We show that MCA in LaFeAsO, $BaFe_2As_2$, and NaFeAs is a non-monotonous function of the exchange splitting of Fe d states. For large values of the splitting the out-of-plane MCA is stronger. However, for sufficiently small exchange splittings the order of the MCA energies is reverted: in agreement with the experiment the in-plane ab anisotropy becomes stronger.