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Role of covalent Fe-As bonding in the magnetic moment formation and exchange mechanisms in iron-pnictide superconductors KIRILL BELASHCHENKO, University of Nebraska-Lincoln, VLADIMIR ANTROPOV, Ames Laboratory — The electronic origin of the huge magnetostructural effect in layered Fe-As compounds is elucidated using LiFeAs as a prototype. The crucial feature of these materials is the strong covalent bonding between Fe and As, which tends to suppress the exchange splitting. The bonding-antibonding splitting is very sensitive to the distance between Fe and As nuclei. We argue that the fragile interplay between bonding and magnetism is universal for this family of compounds. The exchange interaction is analyzed in real space, along with its correlation with covalency and doping. The range of interaction and itinerancy increase as the Fe-As distance is decreased. Superexchange makes a large antiferromagnetic contribution to the nearest-neighbor coupling, which develops large anisotropy when the local moment is not too small. This anisotropy is very sensitive to doping.

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