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Electronic Structure of Mn in III-V semiconductors: lessons from First-principles theory[1]

ALEX ZUNGER, NREL

Early model-theories have suggested that Mn in the III-V semiconductors such as GaAs and GaN will introduce a host-like-hole state that will interact via RKKY-type coupling with the Mn local moment to produce the observed ferromagnetism (FM).This widely publicized model made then specific predictions thus prompting a worldwide search for host materials satisfying these conditions.I will show how modern first-principles electronic structure therory can be used to establish if the basic properties of Mn and other 3d impurities in III-V semiconductors are indeed similar to what was widely assumed in earlier phenomenological model theories.Surprizingly,such calculations (via LDA,GGA,and LDA+U) reveal that the hole induced by Mn is not host-like,and that the ensuing FM is not RKKY-like,but has a characteristic dependence on the lattice-orientation of the Mn-Mn interactions in the crystal which is unexpected by RKKY.I will describe the chemical trends as the host is altered (GaN/GaP/GaAs/GaSb and Chalcopyrite semiconductors such as CuInSe2);as the impurity is altered along the 3d series,and as the Fermi level is altered (via doping).The effects of clustering of impurities,as well as the site-preference (substitutional,interstitial) will be revealed.These calculations open the way to "Inverse Design",by searching the atomic configuration of Mn in the lattice having the highest FM Tc.See Mahadevan,Sarma,and Zunger,Phys.Rev.Letters 93,177201 (2004) .

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