Carrier Induced Ferromagnetism in II-IV-V2 Mn-doped Chalcopyrites

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Although it has been suggested that high T_c dilute magnetic semiconductor (DMS) materials can be realized from common III-V semiconductors doped with Mn, solubility of Mn is limited in these materials and consistently high Curie temperatures have yet to be realized. As an alternative potential route to high T_c materials, we have performed a systematic investigation of the \mathrmII-IV-V_2 alloys doped with Mn, such as (Cd,Mn)GeP_2 and (Zn,Mn)SnAs_2. These ``virtual III-V'' chalcopyrite alloys are compatible with many existing III-V technologies, yet the Mn solubility is greatly increased, because Mn^2+ ions readily substitute on the group II sites. Using density functional calculations we have calculated the ferromagnetic coupling (J) between various configurations and charge states of Mn atoms as well as their solubility, including several intrinsic defects. Here we report that Zn-Sn based compounds have larger ferromagnetic interactions than in \mathrmCdGeP_2 and \mathrmZnGeP_2, which have been grown by several groups. Although the magnitude of the interaction strongly depends on the Mn complexes considered, the larger effective exchange interaction in, e.g., \mathrmZnSnAs_2 and \mathrmZnSnP_2 should result in concomitantly enhanced Curie temperatures. We recommend that this class of materials should be more thoroughly investigated for potentially viable spintronics materials.

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