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Band structure model of magnetic coupling in II-VI and III-V semiconductors SU-HUAI WEI, GUSTAVO M. DALPIAN, National Renewable Energy Laboratory — Mn-doped II-VI and III-V diluted magnetic semiconductors (DMS) exhibit a wide range of magnetic ordering behavior. For example, Mn doped II-VI semiconductors are mostly having antiferromagnetic (AFM) ground state, whereas Mn doped III-V semiconductors are mostly having ferromagnetic (FM) ground state. More interestingly, Mn doped GaN can be either FM or AFM, depending on the Mn concentration, carrier density, or pressure. It has been a great challenge to understand the mechanism of magnetic coupling in these systems. Several models have been used to explain the phenomena, including the Zener/RKKY model, super exchange model and double exchange models. Although these models are successful in explaining some of the systems, they often lack the universality and transparency, and is difficult to compare directly with the band structure calculations. In this work, we will present an unified model to explain magnetic ordering in Mn doped semiconductors. This model is based on the p-d and d-d level repulsions between the Mn ions and host elements and can successfully explain magnetic ordering observed in all Mn doped II-VI and III-V semiconductors such as CdTe, GaAs, ZnO and GaN. This model, therefore, provides a simple guideline for future band structure engineering of magnetic semiconductors.

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