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Heitler-London Model for Acceptor-Acceptor Interactions in Doped Semiconductors KYLE CASTORIA, ADAM DURST, Hofstra Univ, R. N. BHATT, Princeton Univ — The interactions between acceptors in semiconductors are often treated in qualitatively the same manner as those between donors. Acceptor wave functions are taken to be approximately hydrogenic and the standard hydrogen molecule Heitler-London model is used to describe acceptor-acceptor interactions. But due to valence band degeneracy and spin-orbit coupling, acceptor states can be far more complex than those of hydrogen atoms, which brings into question the validity of this approximation. To address this issue, we develop an acceptor-acceptor Heitler-London model using single-acceptor wave functions of the form proposed by Baldereschi and Lipari, which more accurately capture the physics of the acceptor states. We calculate the resulting acceptor-pair energy levels and find, in contrast to the simple singlet-triplet splitting of the hydrogen molecule, a rich ten-level energy spectrum. Our results, computed as a function of inter-acceptor distance and spin-orbit coupling strength, suggest that acceptor-acceptor interactions can be qualitatively different from donor-donor interactions, and should therefore be relevant to the magnetic properties of a variety of p-doped semiconductor systems.

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