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Interactions between native point defects in ZnGeP₂.¹

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Case Western Reserve University — First-principles calculations of the native point defects V_{Zn} , V_{Ge} , Zn_{Ge} and Ge_{Zn} show that under Zn-poor conditions, the dominant defects are the Ge_{Zn} and V_{Zn} . Since these are respectively a donor and an acceptor, one may expect them to attract each other. The formation of complexes of the type $V_{Zn} - Ge_{Zn} - V_{Zn}$ was studied and found to be favorable. A simple molecular model is proposed for the electronic structure of this complex. Optical excitation of electron paramagnetic resonance (EPR) studies by Gehlhoff et al. [1] were used by these authors to extract energy levels in the gap associated with these defects. The model proposed by these authors assumes that the Ge_{Zn} EPR centrum in irradiated samples becomes activated by a two step process in which an electron from a V_{Zn}^{2-} is optically excited to the conduction band and subsequently trapped at a Ge_{Zn}^{2+} site converting the two defects in EPR active sites V_{Zn}^{-} and Ge_{Zn}^{+} . We instead propose a direct transition between the two defect states without the intervening conduction band and show that our calculated occupation energy levels agree with such a model. The V_{Ge} on the other hand is found to have a high energy formation and to be unstable towards the formation of a V_{Zn} and a Zn_{Ge} antisite. [1] W. Gehlhoff, R. N. Pereira, D. Azamat, A. Hoffmann, and N. Dietz, *Physica B* **308-310**, 1015 (2001).

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