Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Interactions between native point defects in $ZnGeP_2$.[1] XIAOSHU JIANG, M. S. MIAO, WALTER R. L. LAMBRECHT, 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).

[1]Supported by AFOSR

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Date submitted: 01 Dec 2004 Electronic form version 1.4