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Does the zinc vacancy in ZnGeP_2 exhibit a Jahn-Teller distortion?¹ WALTER R.L. LAMBRECHT, XIAOSHU JIANG, M.S. MIAO, Case Western Reserve University, SUKIT LIMPIJUMNONG, Suranaree University of Technology — The Zn-vacancy is one of the dominant defects in ZnGeP_2 . Its single negative charge state is EPR active. The hyperfine splitting shows that the unpaired electron is primarily localized on a pair of P atoms. In contrast, first-principles 64 atom supercell calculations using both the FP-LMTO and the VASP method of the V_{Zn}^- state show that the defect maintains S_4 symmetry with the wave function spread equally over 4 P atoms. Here a group-theoretical analysis is presented. When including only the nearest neighbors, the system has D_{2d} symmetry. While the one electron state of the unpaired electron is non-degenerate, a doubly degenerate e -state lies only about 10 meV below it. We show that a P-pairing distortion mode splits this e -state in two states which are even with respect to one of the mirror-planes and odd with respect to the other and thus can only contain two of the P-dangling bonds. Calculations in which a pairing of P atoms is enforced while relaxing the remaining atoms confirm this model. Remaining puzzling aspects of this defect will be discussed.

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