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Identification of a N-related shallow acceptor and related EPR center in ZnO: N2 on Zn site[1] WALTER R.L. LAMBRECHT[2], CWRU, ADISAK BOONCHUN, NIMS, Tsukuba, Japan and Kasetsart Univ., Bangkok — While the deep level of N_O makes it unsuitable for p-type doping of ZnO, a shallow level at about 165±40 meV above the VBM related to N is known to exist in ZnO (Zeuner et al. 2002). Here we show that a N_2 molecule on the Zn site behaves as a shallow acceptor. First-principles calculations show that when N_2 is placed on a Zn site, two electrons are removed from the σ_g^+ HOMO. The molecular levels line up with the ZnO band strucure in such a way that the σ_g^+ level forms a resonance near the VBM. In contrast, for N_2 on the O-site, two extra electrons occupy the π_g LUMO of the N_2 molecule and form a donor level. The 0/- transition level of the acceptor is found at ∼0.2 eV above the VBM. When singly occupied the defect corresponds to a N_2^+ radical. We show that the g-factor, calculated within a simple tight-binding model, of this radical agrees better with an observed EPR center by Garces et al. (2003) than the N_2^- radical. The σ_g nature of the defect wavefunction for N_2 on Zn is consistent with a significant isotropic hyperfine interaction, while the π_g character of N_2 on O is not. The lower value of A_{iso} compared to the isolated molecule is consistent with the shallow nature of the defect.

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