Abstract Submitted
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The impact of +U term on the electronic structure of Mn and Fe ions and of the gallium vacancy in GaN: GGA+U calculations[1] PIOTR BOGUSLAWSKI, OKSANA VOLNIANSKA, TOMASZ ZAKRZEWSKI, Institute of Physics PAS — Band structure of solids is commonly calculated in the Local Density Approximation or the Generalized Gradient Approximation to the Density Functional Theory. Their known failure is the underestimation of the band gap. Within LDA or GGA, the approach of semi-empirical character that leads to correct band gaps consists in adding the +U term for particular atomic orbitals. While the impact of the +U term on bands of an ideal crystal was extensively discussed, its impact on the electronic structure of defects is less understood. Here, we systematically analysed how the +U term affects the properties of the gallium vacancy V:Ga, and of the Mn and Fe transition metal (TM) ions in GaN. The +U term was treated as a free parameter, and it was applied to p(N) and d(TM) orbitals. The results of GGA+U calculations were compared to available experimental data. U(N)=4 eV reproduces well the gap of GaN. We find that the +U terms strongly affect the electronic structure of Mn, Fe, and V:Ga. Surprisingly, however, for U=0, the energies of the gap levels induced by these centers, and of the intra-center optical transitions, agree well with experiment. In contrast, for U(N)=U(TM)=4 eV, these energies are in substantial disagreement with experimental values by about 1-2 eV.

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