Electronic propeties V:Ga-O:N center in GaN and GaInN: GGA+U approach

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Defect complex consisting of cation vacancy and substituting oxygen for N (VO) in GaN [1] is one of the most promising systems for the realization of qubits in semiconductors. Here we analyzed the electronic properties of charged VO in bulk wurtzite GaN and Ga1-xInxN for x ranging from 0 to 0.1 by GGA +U approach [2,3], including the Hubbard-like term +U applied on p(N) and p(O) orbitals. The VO is in high spin state with spins of 1/2, 1 and 3/2 for -1, 0 and +1 charge state, respectively, for both GaN and GaInN. Our calculations of transition levels of -2/-1 and -1/0 transitions in GaN amount to 1.5 and 1.1 eV relative to the VBM, respectively, which is in line with experiments [1]. Finally, we analyzed the possibility of using VO center in GaN and in GaInN in the context of spin qubit operation.

References:

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The work was supported by the NSC (Poland) Grant No. 2015/17/D/ST3/00971. Calculations were done at ICM, University of Warsaw