Electric and magnetic properties of Mn-dimers on zb-GaN/ zb-SiC(001) interfaces

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It has been reported that zinc-blende (zb) phase of the nitrides forms during the growth onto the (001) surface of cubic SiC substrate [1]. Recently, those interfaces have been mostly considered from the side of theirs microelectronics applications [2]. Nowadays, increasing interest in various systems for spintronic applications paves the way to consider the Mn dimers diluted onto the GaN /SiC interface from the point of view of its properties relevant for spintronics. Therefore, in this communication, we focus on Mn dimers diluted onto the SiC/GaN interface considering both its magnetic and electronic properties.

We examine a [Si,Ga] type and [C,N] type GaN/SiC(001) interface with single mixed layer and c(2x2) lateral arrangement predicted to be the most stable in comparison to abrupt and two-mixed interfaces [3]. The mixed layers (co-doped with Si, N, C, Ga atoms) are constructed in such manner to be non-polar on the average, in other words to contain the same number of donor- and acceptor-like bonds. Then, we placed the Mn-atoms at the all non-equivalent substitutional cationic positions at the interfaces, and optimized the all positions of atoms that are in close vicinity of magnetic ions. Further, the stability of arising structures has been investigated. The Mn ions substituted into group III or group IV cationic sites have nominally various charge state (valency). We investigate the influence of the valencies of the Mn ions constituting the Mn-dimers on the magnetic properties of the Mn pairs, in particular the exchange coupling *J* constant. Moreover, the role of the local macroscopic electric field is also considered, by studying the abrupt polar interfaces (i.e., with no mixed layers and with electric charge accomodation).

All of the considered structures have been calculated in the framework of the density functional theory (DFT), with the generalized gradient approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) [4] form of the exchange-correlation density functional as implemented in the numerical package SIESTA [5].

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