

# First-principles study of energetics and magnetic interaction of Mn dimers on heteropolar zb-SiC/zb-GaN(001) interfaces

M. Popielska<sup>1</sup>, M. Sznajder<sup>2</sup>, and J. A. Majewski<sup>1</sup>

<sup>1</sup>*Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warszawa, Poland*

<sup>2</sup>*Faculty of Mathematics and Natural Sciences, University of Rzeszow, Pigoia 1, 35-959 Rzeszow, Poland.*

Interfaces between III-V and group-IV materials are widely studied since 25 years. The numerous studies of the GaN layers grown onto silicon carbide substrate have been reported so far. It is well known that the wurtzite structure is an equilibrium bulk phase of nitrides. Nevertheless, the zinc blende phase of the nitrides is a considerable interest as well, because it forms during growth onto the (001) surface of cubic SiC substrates [1]. Those systems have been mostly considered from their potential microelectronics applications [2]. In recent years, there has been the increasing interest in possible spintronic applications, therefore, in this communication we focus on Mn dimers diluted onto the SiC/GaN interface from the point of view of its properties relevant for spintronics.

To investigate energetics and magnetic interactions of Mn dimers at the SiC/GaN interfaces, we decided to perform extensive *ab initio* studies in the framework of density functional theory (DFT), with the generalized gradient approximation (GGA) to the exchange-correlation density functional in the form proposed by Perdew-Burke-Ernzerhof (PBE) [3] and norm-conserving separable pseudo-potentials to describe electron-ion interaction, as implemented in the numerical package *SIESTA* [4]. We focus on the polar and non-polar intermixed (co-doped with Si, N, C, Ga atoms) interfaces between zinc blende SiC substrate and strained zinc blende GaN. We placed two Mn-atoms at the all non-equivalent substitutional positions at the interface, and at the monolayers directly attached to the interface. The positions of the atoms at the 4ML from up and down of interface have been fully relaxed until forces acting on them converge to less than 0.02 eV/Å, whereas the rest of the atoms (i.e., 8MLs) has been kept fixed. Our results show that the energy differences between the all possible configurations of Mn dimers at interface and close to the interface are in the range of (0.2 – 27.3) meV/Å<sup>2</sup> per atom.

We investigate the role of the different valency of Mn ions constituting the dimer (owing to their different surroundings) on the magnetic interactions between Mn pairs, in particular on the magnitude of the exchange coupling  $J$ . Moreover, in the case of the polar abrupt interfaces (which originate from their heterovalent character of two materials) the influence of the macroscopic electric field on the magnetic and energetic properties of Mn pairs can be also investigated.

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