Theoretical investigation of contact-induced phenomena in composite materials containing fullerenes and nanotubes deposited on ferromagnetic substrates

Exploring new spin filtering materials is an important issue of modern spintronics. Conducting spin-polarized current, these materials may be implemented in magnetoresistive memory elements, hard disk scanning heads, and other devices. Previously it was shown that planar hexagonal nanostructures such as graphene and *h*-BN have great potential for being used in spintronic devices due to the spin polarization induced by the contact with ferromagnetic substrate. It is reasonable to suppose that boron nitride and carbon nanotubes (BNNTs and CNTs) can also be used for this purpose. Although the contact interaction of carbon and BN nanotubes with ferromagnetic substrates is supposed to be quite similar to that of the corresponding graphene and *h*-BN hexagonal monolayers, which can be considered as nanotubes of extremely large diameter, finite thickness of the tubes can result in a significant change of interface properties. This effect has not been investigated in detail.

The interaction of zigzag and armchair carbon and boron nitride nanotubes (NT) with ferromagnetic transition metal (TM) surfaces, namely, Ni(111) and Co(0001), was studied within the framework of density functional theory. Different configurations of composite compartments mutual arrangement were considered. All NT(n,0)/Co interfaces were found to be more energetically favorable than NT(n,0)/Ni, and conductive carbon nanotubes demonstrate slightly stronger bonding than semiconducting ones. Partial densities of states and spin density spatial distribution of optimized structures were investigated. Influence of ferromagnetic substrate on nanotubes' electronic properties was discussed. The presence of contact-induced spin polarization was established for all nanocomposites. The contact-induced polarization of BNNT resulted in the

appearance of local conductivity in the vicinity of the interface while the rest of the nanotube lattice remained to be insulating.

Organic-based spintronics is one of the most fast-developing fields in nanoelectronics. Buckminsterfullerene-based composites are widely investigated due to their unique properties and there are a number of studies on their interaction with various types of substrates. Ferromagnetic surfaces are of a particular interest for potential spintronics applications. Based on the data reported in literature, one can suppose that there is more than one stable structure in C_{60}/Fe(001) composite system. Different possible adsorption sites of C_{60} molecule were investigated revealing the possibility of their coexistence and its influence on the composite properties.

Half-metallic $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) is widely used in spintronic devices due to its high spin polarization. It has a lot of advantages comparing with conventional ferromagnetic materials (e.g. Fe, Co, Ni) which are much less spin polarized and suffering from well-known conductivity mismatch problem. Using half-metallic electrodes (LSMO) allows achieving up to 95% contact spin polarization in MTJ devices without using any additional layers. Moreover, in contrast to the above mentioned transition metals, LSMO is highly resistive against oxidation. These features make LSMO an ideal candidate to be used in spintronics.

Atomic and electronic structures of LSMO-based composites with carbon nanotubes were studied within the framework of density functional theory with respect to the termination of LSMO surface. The deformation of tubes caused by the lattice mismatch with the substrate resulted in a major change in their electronic structure. The surface terminated with Mn-O layer provided much stronger interaction with carbon nanotubes than Sr-O terminated one did. The interaction with transition metal atoms was essential for forming nanocomposites when nanotube structure was visibly distorted.

Spinterface between fullerene C_{60} and $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) was studied within the framework of density functional theory. As previously, co-existence of many different configurations was shown, and probabilities of their appearance

were estimated. Dependence of composite properties on configuration and temperature was also investigated. Key role of transition metal atoms in both binding between composite compartments and magnetic ordering in C_{60} molecule was discussed. The latter was suggested to be responsible for spin-polarized charge transport while overall magnetic moment of fullerene molecule was relatively small.