Investigation of the interaction of iron oxide with carbon nanotubes

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Methods and materials. Computer modeling was provided within the density functional theory on the B3LYP/6-31G level. Firstly, optimized geometries of molecular clusters of “armchair” (6,6) carbon nanotube (CNT), “zigzag” (6,0) carbon nanotube and iron oxide (II,III) were obtained. Pending bonds at cluster boundaries were closed by pseudo-atoms, which are hydrogen atoms. The process of interaction of such nanotubes with iron oxide (II,III) was modeled by the reaction coordinate change method while the molecule of oxide approaches to the surface of nanotube along the perpendicular to the nanotube longitudinal axis that passes through the chosen positions on the surface. We considered approaching to the three positions on the surface: to the carbon atom, the middle of the bond and the centre of the hexagone. Results of calculations enable us to draw energy curves which illustrates considered interaction and define the distance between the molecule and nanotube at which the chemical bond formed (minimum of the potential energy). We optimized structures corresponding to the point of the minimum of the potential energy and investigate the electronic properties of complexes CNT+Fe3O4. Value of an energy gap E_g was calculated as difference of the energy of the energies of the lowest unoccupied molecular orbital E_{LUMO} and highest occupied molecular orbital E_{HOMO}. Visualization of the density of states (DOS) provided with the program GaussSum.

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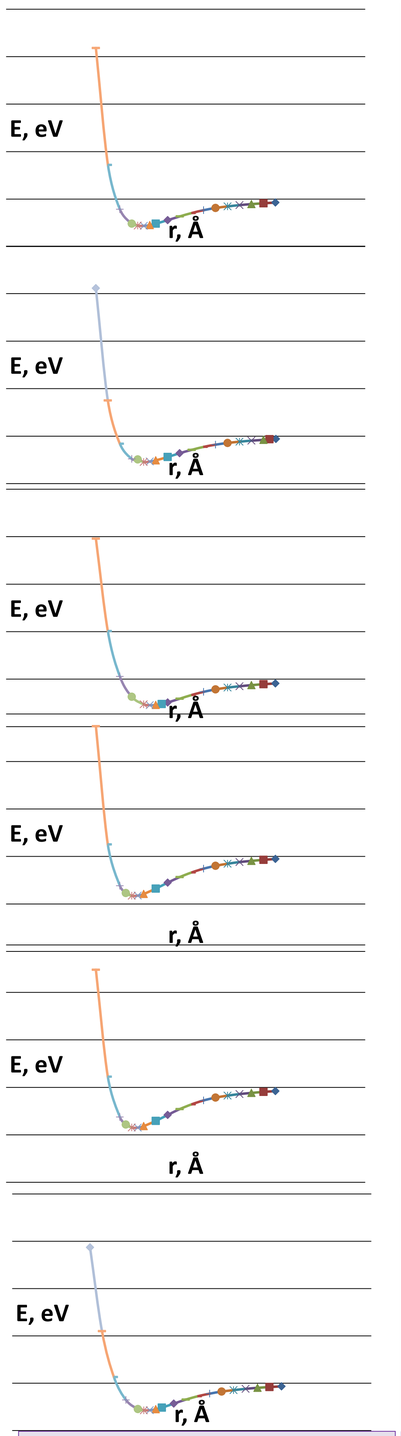
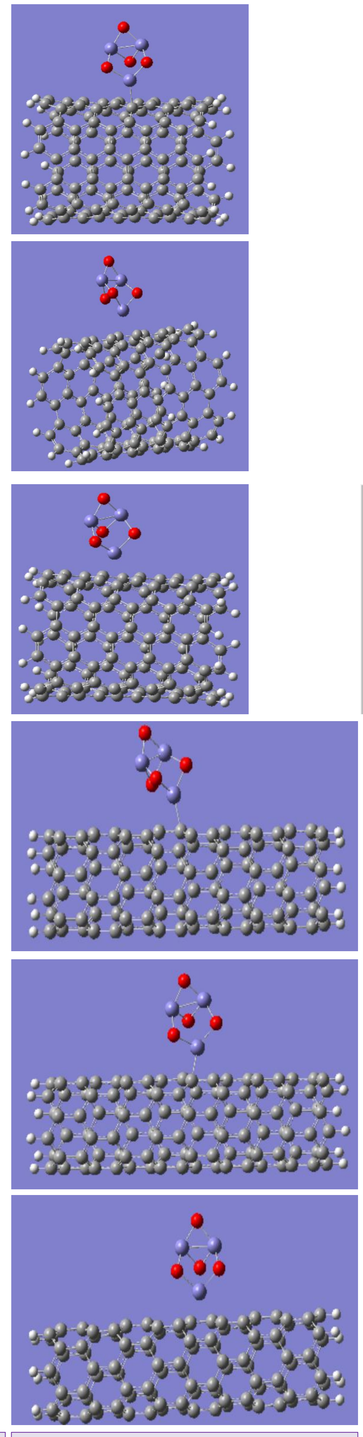
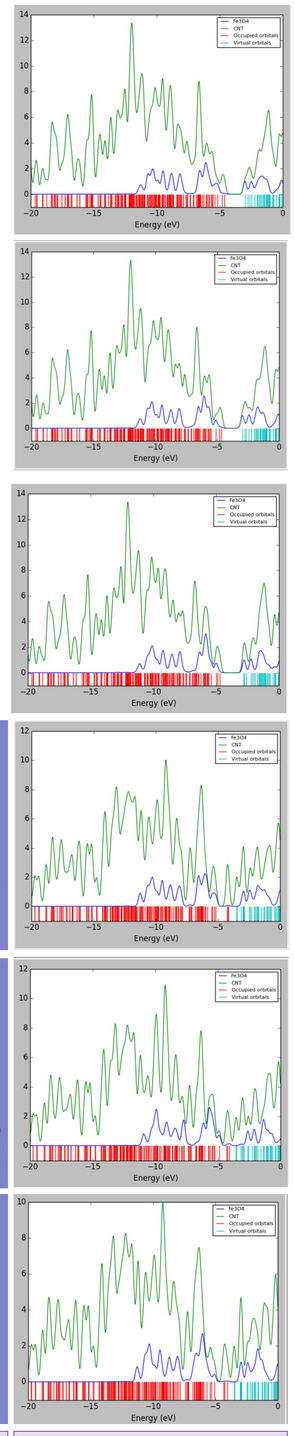


Energy curves for the approaching to the carbon atom, the middle of the bond, to the centre of hexagone for CNT (6,6) and for CNT (6,0) respectively.



Optimized geometries of CNT+Fe3O4 complexes.



DOS functions (green) and contributions to them by oxide (blue).

Complex	E_g, eV
CNT(6,6) (pure)	1,889
CNT(6,6)+Fe3O4 (to the atom)	1,644
CNT(6,6)+Fe3O4 (to the middle of the bond)	1,699
CNT(6,6)+Fe3O4 (to the centre of the hexagone)	1,909
CT(6,0) (pure)	0,449
CNT(6,0)+Fe3O4 (to the atom)	0,665
CNT(6,0)+Fe3O4 (to the middle of the bond)	0,507
CNT(6,0)+Fe3O4 (to the centre of the hexagone)	0,546

Conclusion. In the present work we found points corresponding to the minimum of potential energy in the interaction of CNTs with Fe3O4, obtained optimized structures of such complexes and define their electronic properties. We conclude that interaction between chosen types of CNTs and iron oxide (II, III) take place in all considered positions. Distance to the surface of CNT from the closest Fe atom amounts 2,3-2,4 for C(6,6) nanotube and 2,1-2,2 for the C(6,0) nanotube. We can see that influence of an addition of iron oxide (II, III) on the energy gap value is different and depends on the type of nanotube and position of addition. In the case of “armchair” nanotube E_g rises for all complexes with Fe3O4, but approaching of oxide to the carbon atom of surface has the strongest influence on this value. In the case of “zigzag” nanotube E_g decreases if the approaching is to the atom or to the bond, but addition of oxide to the centre of hexagone leads to the rising of energy gap.