The influence of metal oxide nanoparticles on the energy and electrophysical characteristics of quasi-2D graphene-nanotube film

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The aim of this study

Investigation of the electrophysical properties of hybrid quasi-2D carbon films in the presence of metal oxide nanoparticles. The hybrid carbon films are formed by graphene sheets and vertically oriented single-walled carbon nanotubes. Aluminum, titanium, and hafnium oxides are considered as part of the metal oxide.

Methods and approaches

The optimization of the atomic structure was carried out using the Density Functional based Tight Binding (DFTB) method.The Fermi level was determined from band structure calculations performed using the DFTB method. Electrical resistance and conductivity were calculated within the Landauer-Buttiker formalism using the nonequilibrium Green's function method.

Conclusions

Patterns in the influence of metal oxides on the Fermi level and resistance/conductivity of graphene-SWCNT structures were identified. It was found that, compared to the Fermi level of the graphene-SWCNT structure, the Fermi level of the graphene-SWCNT/Al2O3 interface shifted downward along the energy axis. For the graphene-SWCNT/TiO2 and graphene-SWCNT/HfO2 interfaces, the Fermi level shifted upward along the energy axis compared to the Fermi level of the graphene-SWCNT structure. The difference in the behavior of the Fermi level between the interfaces is explained by the difference in the direction of charge transfer between the carbon framework and the metal oxide: in the case of the graphene-SWCNT/Al2O3 interface, the carbon framework donates a charge to the metal oxide, while in the other two cases, it accepts it. The graphene-SWCNT/Al2O3 interface resistance is 43 kOhm and the conductivity is 0.02 mS, remaining in the same order of magnitude as for the graphene-CNT structure (resistance 14.7 kOhm and conductivity 0.07 mS). The graphene-SWCNT/TiO2 and graphene-SWCNT/HfO2 interface resistances are 28 kOhm and 53 kOhm, respectively, and the conductivities are 0.03 mS and 0.03 mS, respectively.

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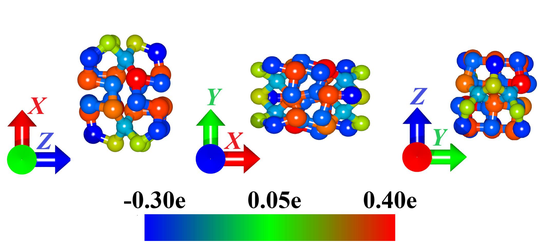
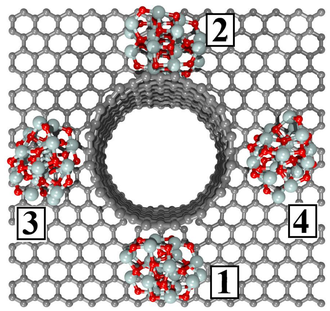
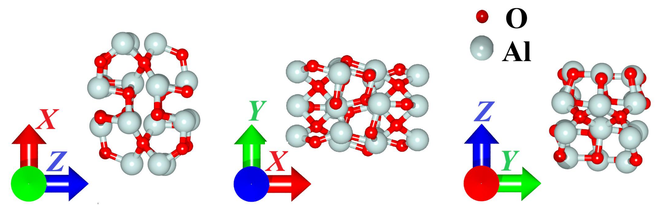


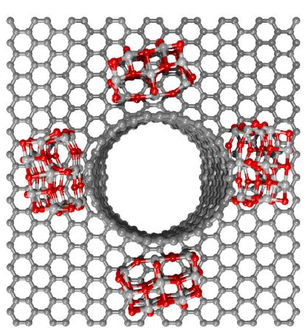
Atomic cluster Al_2O_3: charge redistribution



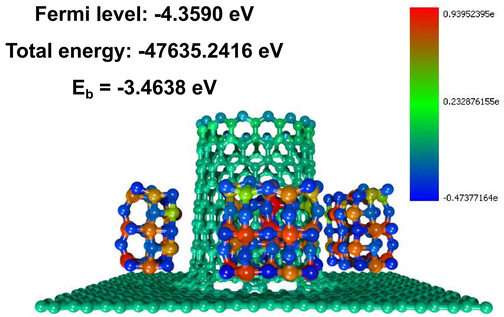
graphene-SWCNT hybrid with 4 Al2O3 nanoparticles



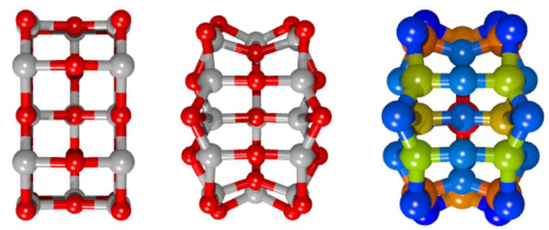
Atomic cluster Al_2O_3: atomic structure



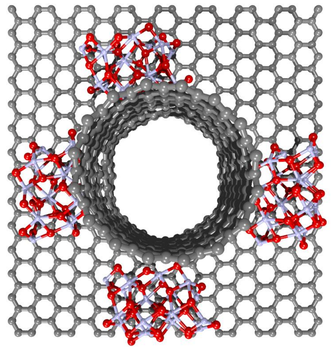
graphene-SWCNT hybrid with 4 TiO2 nanoparticles



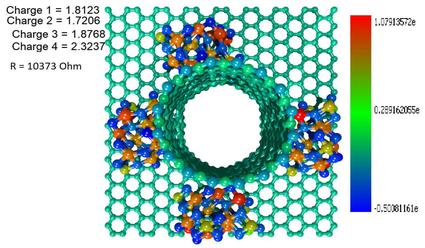
Charge redistribution in system graphene-SWCNT hybrid/Al2O3



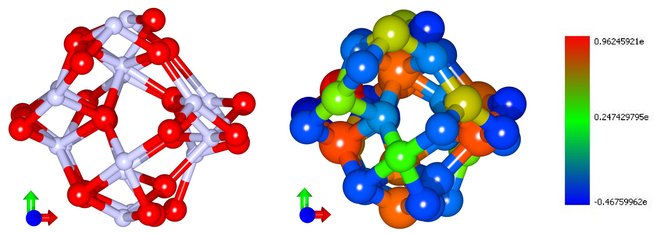
Atomic cluster TiO_2: atomic structure and charge redistribution



graphene-SWCNT hybrid with 4 HfO2 nanoparticles



Charge redistribution in system graphene-SWCNT hybrid/HfO2



Atomic cluster HfO_2: atomic structure and charge redistribution