



Tunneling Current Control in Graphene-Nanotube Structures

Michael M. Slepchenkov¹, Dmitry A. Kolosov¹, Olga E. Glukhova^{1,2};

¹Saratov State University, Saratov, Russia;

²I.M. Sechenov First Moscow State Medical University, Moscow, Russia



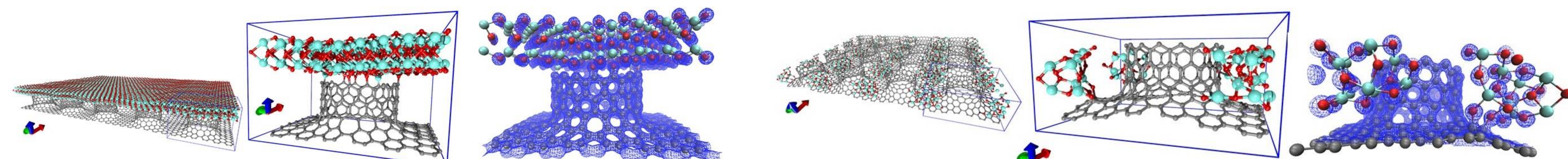
Aim of the study

This study employs the SCC-DFTB method to investigate hybrid carbon films composed of seamlessly interconnected graphene nanosheets and vertically aligned single-walled carbon nanotubes (SWCNTs). It analyzes the potential use of such films as conductive channels in field-effect transistors, where conductivity is modulated by depositing metal oxide nanoparticles onto the carbon film. Furthermore, the study explores methods to control leakage current at the interface between the quasi-2D graphene-CNT conductive channel and the aluminum oxide (Al_2O_3) dielectric by varying the dimensionality of the latter—specifically, comparing 2D and 0D Al_2O_3 structures in contact with the hybrid carbon film.

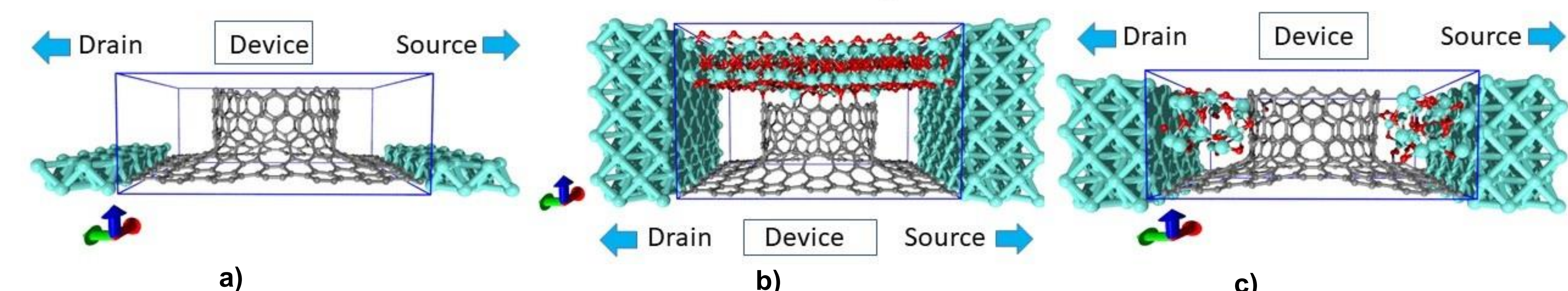
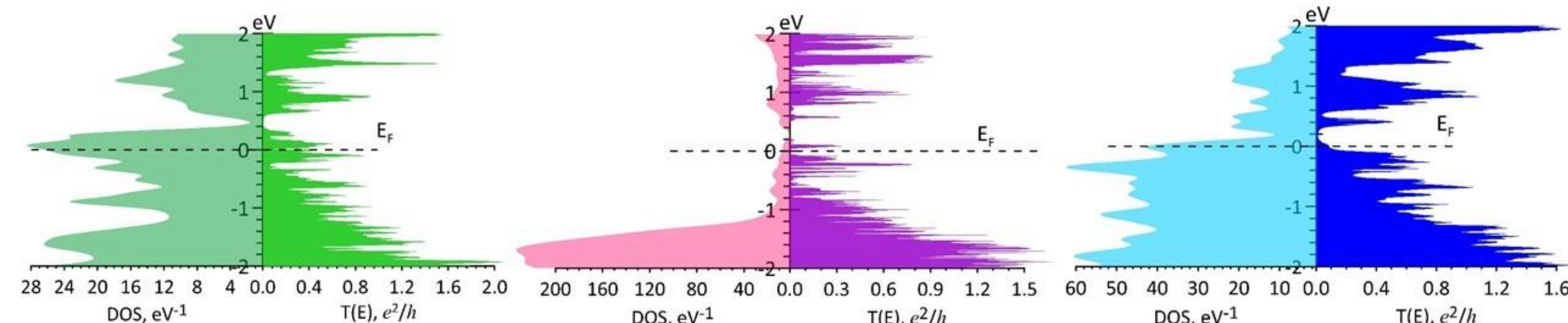
Conclusions

The electrical conductivity properties of quasi-2D films within graphene-CNT/2D- Al_2O_3 and graphene-CNT/0D- Al_2O_3 interfaces were investigated using the SCC-DFTB method (self-consistent charge density functional tight-binding). The leakage current at the interface between the carbon nanomaterial and the dielectric oxide film was calculated. It was determined that the dimensionality of the Al_2O_3 component plays a decisive role in the electronic structure and transport properties of graphene-CNT/ Al_2O_3 interfaces. It was shown that Al_2O_3 in the form of a 2D film creates a more effective dielectric barrier compared to 0D Al_2O_3 nanoparticles, resulting in a significant reduction in electrical conductivity across the barrier and a decrease in leakage current in the "graphene-CNT + Al_2O_3 " channel. Conversely, the graphene-CNT/0D- Al_2O_3 system retains higher conductivity due to the presence of conductive pathways at the graphene-CNT/ Al_2O_3 interface. The results demonstrate the feasibility of controlling leakage current in structures based on graphene-CNT/ Al_2O_3 composite films by modifying the morphology of the dielectric layer.

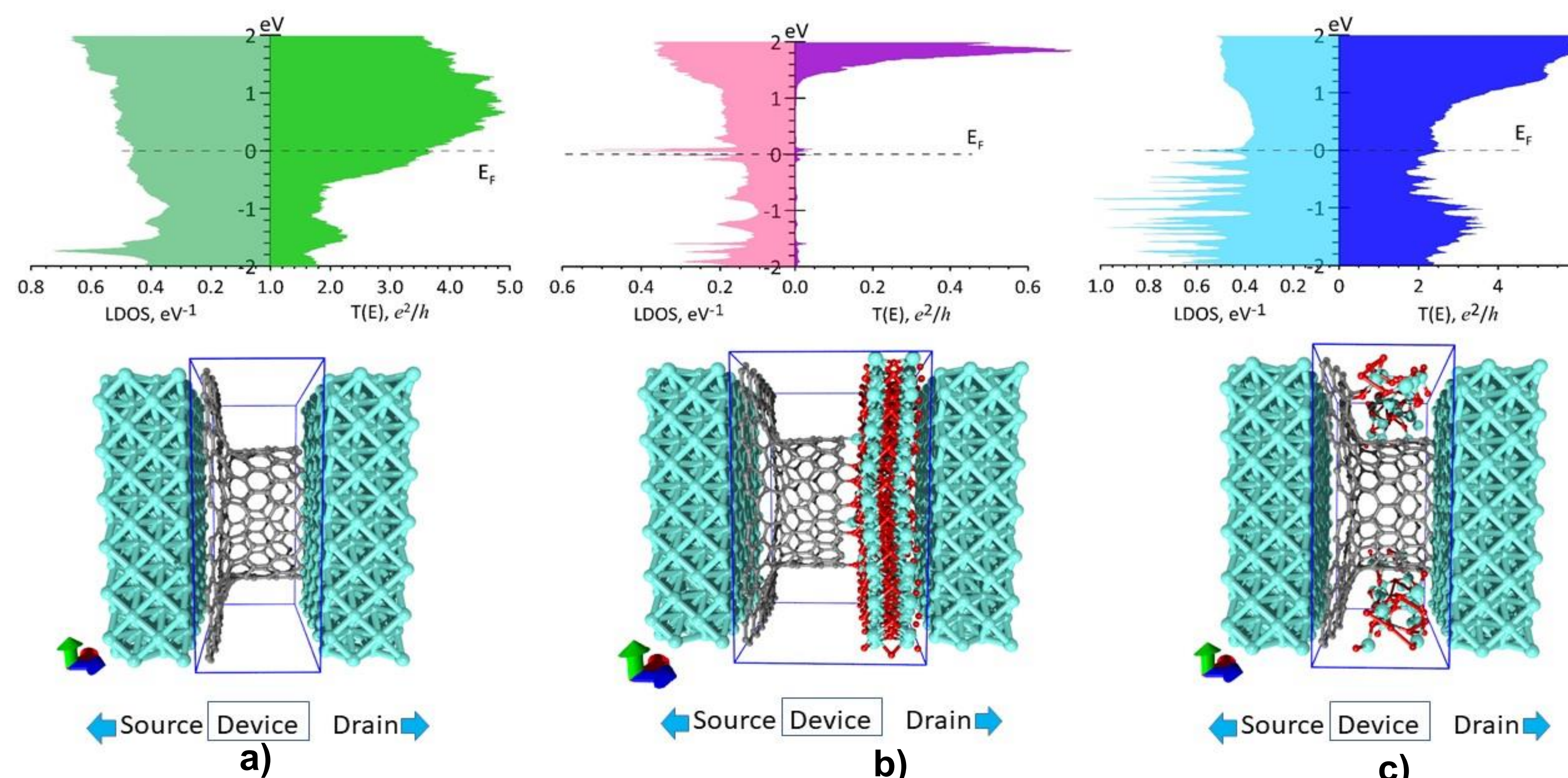
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Atomic structures and isosurfaces with an electron charge of 0.15e for quasi-2D film models 2D-I (left) and 2D-II (right). Aluminum atoms are colored cyan, oxygen atoms red, and carbon atoms gray.



Planar conductivity properties of a graphene/CNT film (Al electrodes): a) schematic of the graphene/CNT contact and DOS/T(E) plots; b) schematic of the 2D-I structure contact and DOS/T(E) plots; c) schematic of the 2D-II structure contact and DOS/T(E) plots.



Vertical conductivity properties of the graphene/CNT film (Al electrodes): a) schematic of the graphene/CNT contact and DOS/T(E) plots; b) schematic of the 2D-I structure contact and DOS/T(E) plots; c) schematic of the 2D-II structure contact and DOS/T(E) plots.

Electrical conductivity was investigated in two directions: longitudinal (along the graphene—the armchair direction) and vertical. The latter allows for the assessment of leakage current at the "carbon framework + Al_2O_3 " interface. To evaluate electrical conductivity, calculations of the transmission function were first performed, serving as the basis for subsequently calculating the conductivity values. The electrical conductivity of the composite film—comprising a graphene-CNT structure and an Al_2O_3 dielectric—was calculated within the framework of Landauer-Büttiker theory. Aluminum films of varying thicknesses were selected as electrodes, depending on the height (along the Z-axis) of the supercell. An analysis of the graphs indicates that the introduction of aluminum oxide leads to a decrease in electrical conductivity—an effect that is more pronounced for the 2D-I film than for the 2D-II film. This is evidenced by the appearance of a gap in the transmission function profile, resulting from a sharp drop in the DOS intensity for this structure.

The vertical conductivity of the films, which determines the presence or absence of leakage current, was investigated in a similar manner. As in the previous case, integral transmission functions $T(E)$ were calculated for the systems "carbon framework + Al electrodes," "carbon framework + 2D-I + Al electrodes," and "carbon framework + 2D-II + Al electrodes." Contact configurations and DOS/ $T(E)$ plots are shown in the figure. In this instance, the Al electrodes were modeled as identical cells, as their dimensions were determined solely by the $X \times Y$ dimensions of the carbon supercell. The integral transmission function for the 2D-I structure exhibits minimal values near the Fermi level, indicating minimal electrical conductivity. For the carbon framework and the 2D-II type film, a relatively high transmission function intensity—in the range of ~3–4 arbitrary units—is observed.