Calculation of electronic and transport properties of single-walled boron nanotubes

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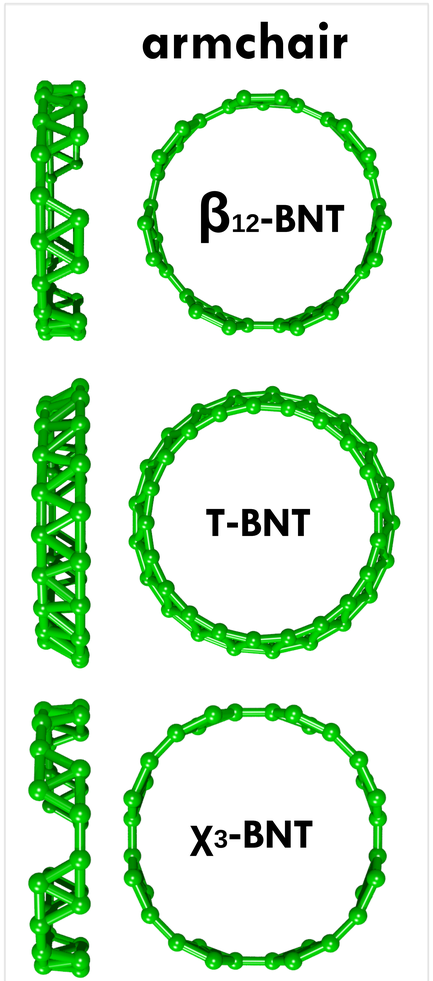
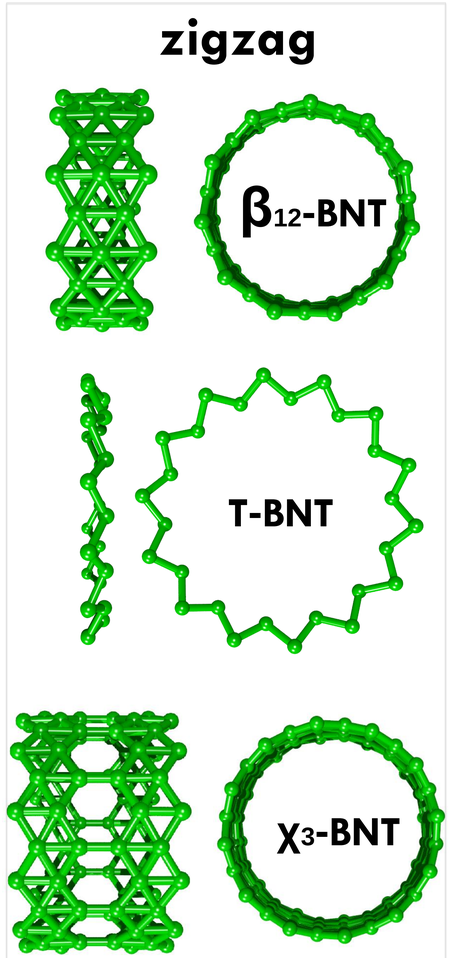
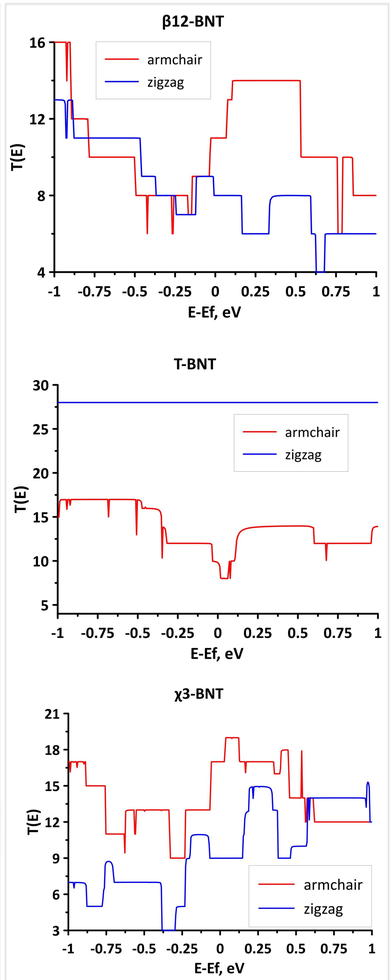
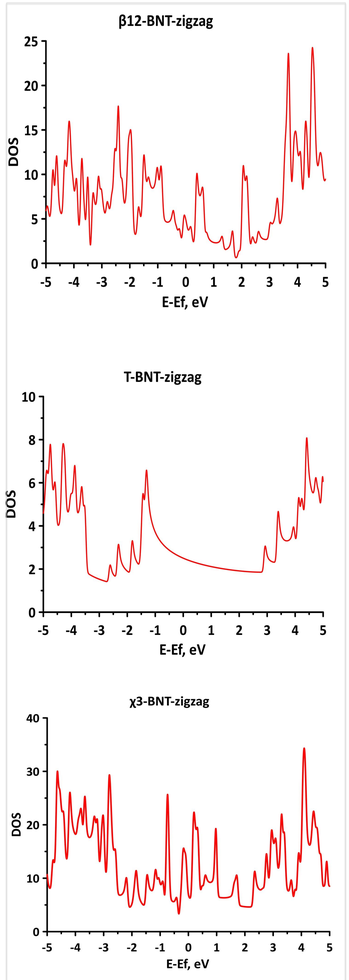
Materials and methods

In this work, the SIESTA 4.1 software package is used for geometry relaxation, searching for the potential energy minimum, and calculating the electronic properties of nanostructures. We used a Density Functional Theory (DFT) base set with Generalized Gradient Approximation (GGA) and Purdue-Burk-Ernzerhoff (PBE) parameterization because these calculation parameters performed well both in terms of calculation accuracy and calculation time. The force acting on each atom after relaxation was set to 0.04 eV/Å, and the energy limit was chosen to be 350 Ry. The Brillouin zone was sampled by a 1 × 1 × 36 Monkhorst-Pack grid. The relaxation process was performed by the Broyden algorithm and the Pulay corrections.









Structure	E[Fermi] zigzag, eV	E[HoF] zigzag, eV	Resistance zigzag, Ohm	E[Fermi] armchair, eV	E[HoF] armchair, eV	Resistance armchair, Ohm
β12-BNT	-5.188	-6.049	1527.4	-5.376	-6.056	1197.1
T-BNT	-5.808	-6.019	457	-5.074	-5.873	1311.5
χ3-BNT	-5.124	-6.034	1404.6	-5.133	-6.030	748.5

Conclusions

In this poster presentation presents equilibrium atomistic models of single-walled boron nanotubes obtained using the first-principles SIESTA code. Atomistic models of boron nanotubes were obtained by twisting monolayer sheets of borophene (triangulated, beta and hi-3 topologies) followed by geometric relaxation of atomic coordinates and translation vectors. The results of the calculation of the density of electronic states (DOS) showed the absence of a band gap for all considered cases, as well as a negative value of the formation energy. At the same time, using the nonequilibrium Green-Keldysh functions, the electron transmission functions were obtained for all the considered structures, where a boron nanotube composed of triangulated borophene in the "zigzag" direction showed an extremely low resistance value equal to 457 Ohm and a formation energy equal to -6.019 eV. This study makes it possible to judge the applicability of boron nanotubes as low-dimensional conductors in nano- and microelectronics.