Supporting online material

Methods

Our electronic structure calculations were performed using the VASP code,[1] which implements the plane wave ultrasoft pseudopotential formalism based on density functional theory (DFT) within the local density approximation (LDA). The plane-wave cutoff was chosen as 286 eV. The quantum transport calculations were performed using the Atomistix ToolKit2.0 package,[2,3] which implements DFT-based real-space, nonequilibrium Green's function formalism. The mesh cutoff of carbon atom is chosen as 100 Ry to achieve the balance between calculation efficiency and accuracy. In the transport calculations, the gating effect is treated theoretically by adding an electrostatic potential equaling to gate voltage to the channel region of the device structure, so the effect of gate geometry is not considered. In all the calculations, the edges of GNRs are saturated with H to remove C dangling bonds. Structural optimizations were first carried out on some structures until atomic forces converged to 0.01 eV/Å. However, we found that the structural optimization does not change considerably the atomic or the electronic structures of GNRS. Thus, to save computational time, we have performed large-scale transport calculations with the fixed edge C-C and C-H bond lengths at the optimized values of 1.409 Å and 1.10 Å, respectively.

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