Contact spacing controls the on-current for all-carbon field effect transistors

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All-carbon field-effect transistors, which combine carbon nanotubes and graphene hold great promise for many applications such as digital logic devices and single-photon emitters. However, the understanding of the physical properties of carbon nanotube (CNT)/graphene hybrid systems in such devices remained limited. In this combined experimental and theoretical study, we use a quantum transport model for field-effect transistors based on graphene electrodes and CNT channels to explain the experimentally observed low on currents. We find that large graphene/CNT spacing and short contact lengths limit the device performance. We have also elucidated in this work the experimentally observed ambipolar transport behavior caused by the flat conduction- and valence-bands and describe non-ideal gate-control of the contacts and channel region by the quantum capacitance of graphene and the carbon nanotube. We hope that our insights will accelerate the design of efficient all-carbon field-effect transistors.

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with technological progress, semiconductor devices are rapidly shrinking in size and conventional silicon systems reach their physical limits. As an alternative, the low-dimensional carbon structures graphene and carbon nanotubes (CNT) have enormous potential for future electronics. Graphene exhibits excellent material properties such as high charge mobility, mechanical strength, transparency, and flexibility. Semiconducting CNTs combine most of the exceptional characteristics of graphene with a direct, structure-dependent bandgap. Both types of nanostructures can be scalably fabricated and integrated as building blocks for electronic devices serving as electrical contacts and channels in carbon nanotube field-effect transistors (CNTFETs). Other promising applications include nanocomposite materials, biosensors, scaffolds for tissue engineering, light emitters, and in particular single-photon sources or photodetectors, respectively. All-carbon ultra-flat, flexible, and transparent graphene/CNT transistors offer outstanding possibilities for fundamental and applied research. The electrical properties of CNTFETs with metallic contacts were extensively studied in previous works. Despite the variety of possible device geometries, the performance of the considered devices was limited due to the inevitable Schottky barriers in the case of chemisorbed metals (e.g., Ti, Ni) and the enhancement of contact resistance upon contact length downscaling in the case of physisorbed metals (e.g., Pt or Sc). The work-function difference between CNTs and graphene is negligible as all-carbon CNTFETs exhibit ambipolar electrical properties which make them particularly interesting for light-emitting devices. Furthermore, graphene is chemically stable, easy to fabricate in large areas using chemical vapor deposition (CVD), and its two-dimensional structure causes weak screening of the gate electric field. However, it has been shown that the electronic properties of the atomistic CNT/graphene system depend critically on the distance between the tube and graphene electrode. Presently, rational design of high-quality all-carbon transistors is constrained by challenges in the fabrication of the devices, requiring site-selective integration of individual CNTs between graphene electrodes which is barely possible using conventional lithography techniques, but is feasible with the help of dielectrophoresis. Nevertheless, Xiao et al. have demonstrated field-effect transistors with graphene/CNT junctions and Scandium drain-electrodes with steep subthreshold-switching properties and high on-state currents. The efforts to understand the CNT-graphene system theoretically encounter obstacles as well. In the past, theoretical studies on transport in CNT-based devices have been conducted using nonequilibrium Green function formalism (NEGF) combined with density functional theory (DFT). Recent studies used the DFT + NEGF method to treat single molecular junctions with carbon-based electrodes. However, simulations of all-carbon transistors with realistic contact and channel sizes remained unfeasible due to the necessity to simulate quantum-mechanical systems comprising thousands of atoms. In the work of Fediai et al., a rigorous method to treat quantum transport through 2D-3D extended contacts, utilizing DFT and NEGF was developed, enabling full quantum transport simulations from first principles. We have adapted this method to a CNT transistor with graphene electrodes, which exhibits 1D/2D junctions. The aim of our work is to understand the fundamental properties of the graphene-CNT junction. We approach this problem through well-defined experiments and atomistic simulations where we developed a dedicated combination of DFT and NEGF specifically for graphene-CNT contacts, based on earlier work. This method pushes the limits of the conventional combined DFT+NEGF methods toward the channel and contact lengths of ≈100 nm so that quantum mechanical treatment of the whole all-carbon transistor becomes feasible. On the experimental side, we fabricated and electrically characterized all-carbon transistors with a structure similar to the simulated atomistic structures in terms of bandgap and channel length. A dielectrophoretic deposition allows precise placement of single CNTs with defined chirality between the electrodes. Using our method, we have analyzed the spectral function of the CNT on top of the graphene to understand the effect of the CNT/graphene spacing on the charge injection and computed the local density of states and band bending in the device at different drain- and gate-source voltages. Hence, the effect of the quantum capacitance of the CNT and graphene was considered to realistically include the electrostatics inside the atomistic channel and contact region. We observe that large CNT/graphene spacing and short channel lengths reduce the current flow through the transistor by approximately three orders of magnitude. The model was validated by comparing it with the measured current-voltage characteristics. The gained insights can assist a rationalization of the design of various devices based on CNTs and graphene electrodes.

**Results and discussion**

**Experimental set-up and simulated system.** The experimental devices and their virtual counterparts were designed to be as similar as technical facilities and computer resources allowed. We fabricated devices that consist of graphene electrodes and preliminary sorted semiconducting CNTs. To this end, CVD-grown graphene was patterned on top of a SiO₂/Si layer using electron lithography to form the electrodes with a channel length of 100 nm. Individual nanotubes that bridged the contacts were suspended from a toluene-based suspension, in which the majority of carbon nanotubes have (9,8) chirality (Fig. 1a). The deposition was performed using ac-dielectrophoresis adapted for the graphene electrodes. Figure 1b shows a scanning electron micrograph of an exemplary device. Afterward, we placed the sample in a continuous-flow cryostat and characterized it under vacuum conditions at 10⁻⁶ mbar. After vacuum annealing at 350 K to remove the remaining water layer, the sample was cooled down and the electrical characterization of the all-carbon transistors was performed at temperatures down to 4 K. Figure 1c shows the simulated atomistic structure of the virtual counterpart of the fabricated devices and denote the contact and channel length, L_contact and L_channel, respectively. To enable the computational feasibility of the developed model, instead of chiral (9,8)-CNTs, we chose (13,0)-zigzag nanotubes, which have a much smaller period but similar bandgap. Since the current-voltage characteristics are mainly governed by the bandgap of the channel material, the use of (13,0)-CNTs is justified (see method section for more details). Figure 1d shows the virtual device we use for the simulations, illustrating the electrodes (source φₛ, drain φₚ, gate φ₉, and the gate voltage V₉). The channel of the model system is 17 nm long, while the contact length is a variable parameter with an arbitrary upper limit. Conventional NEGF + DFT software cannot simulate quantum transport in systems with extended contacts, with an electrode-channel overlap of more than a few Angstrom. Therefore, we have theoretically developed and programatically implemented a dedicated NEGF + DFT method for simulating quantum transport in a transistor with arbitrary graphene/CNT overlap (see methods section).

**Interaction strength between the CNT and graphene electrodes.** The peculiarity of the all-carbon CNTFET is the use of graphene for the source and drain electrodes. A profound understanding of the electrical properties of extended CNT/graphene contacts is necessary to identify potential bottlenecks and, if possible, to circumvent those by designing devices appropriately. We analyze the spectral function A(E,kₙ) to provide information about the energy-momentum relation of the electrons in the all-carbon system. Experimental methods for determining the spectral function, such as angle-resolved photoemission spectroscopy...
(ARPES), apply only to planar systems\textsuperscript{15,46}. Our developed model does not have this limitation, and thus we have computed the spectral function in the part of the tube sitting on the graphene electrode with equation (11) for CNTs with different CNT/graphene spacings, as discussed in detail in the methods section. The geometry files for the CNT/graphene system with different CNT/graphene spacings are provided in Supplementary Data 1. We used the spacing between the graphene and the CNT to mimic the effect of residual polymers helically wrapped around the CNT that remain after the selective deposition processes to obtain monochiral, semiconducting CNTs out of a polychiral suspension\textsuperscript{47,48}. With this, we assume that the residual polymer does not affect the electrical properties of either CNT or graphene. Figure 2 shows the simulated spectral functions for the (13,0)-CNT on top of the graphene layer plotted in a heat map plot. For a large spacing of 5.0 Å (Fig. 2a), sharp and distinct peaks are observed in the spectral function. A reduced spacing (Fig. 2b-d) results in a broadening of the peaks. Even at a distance of 3.0 Å which is smaller than the sum of two carbon van der Waals radii (Fig. 2d), the typical band structure of the carbon nanotube is visible. Hence, we do not expect that the graphene electrode will distort the band structure of the carbon nanotube, even after the removal of the residual polymer. Due to weak graphene/CNT interaction, we expect the current to flow over the entire contact region of the CNT and graphene\textsuperscript{27}. The preservation of the band structure is similar to conventional metallic Pd or Pt contacts. This is in stark contrast to Ni or Ti contacts which destroy the band structure of the CNT upon the contact by “metalizing” it (that is, introducing states in the vicinity of the Fermi level). As a consequence, the Fermi level in the CNT on top of Ti or Ni is pinned near the center of the bandgap leading to the formation of ambipolar Schottky contacts\textsuperscript{27}. We point out that our method is sensitive to the chirality of the carbon nanotube in the gr/CNT junction. For example, (12,0) CNT, remains gapless in contact with graphene (supplementary figure 6).

The efficiency of the bottom gate. Another distinctive feature of the graphene electrodes is that they do not perfectly screen the CNT in the contact region from the electrostatic field of the gate electrode. Consequently, the parts of the CNT sitting above the graphene electrodes can be electrostatically doped by the gate-source voltage \(V_{GS}\). Our considered device is fundamentally different from conventional CNTFETs with metallic electrodes, where the gate electrode controls only the bands in the channel region. To describe the gating efficiency in the center of the channel region and the contacts, we define the gate-induced band shifts \(\xi_{contact}\) and \(\xi_{center}\), respectively. Treating the electrostatics by self-consistently solving the Poisson equation would be numerically too expensive for a model of this complexity. However, to describe the electrostatics realistically, the quantum capacitance \(C_Q\) \textsuperscript{(Eq. (28))} of the graphene-CNT system in the contacts and the channel center was computed and taken into account. The band shift can now be determined by numerically solving the differential equation (27).

\[
\frac{d\phi}{dx} = \frac{C_Q}{\varepsilon_{CNT}} \frac{dV}{dx} + \frac{1}{\varepsilon_{Si}} \frac{dV}{dx} + \frac{1}{\varepsilon_{SiO2}} \frac{dV}{dx} \left( V_{GS} - V_{FT} \right) \left( 1 - \alpha \right) - \frac{1}{\varepsilon_{SiO2}} \frac{dV}{dx} \alpha \left( V_{GS} - V_{FT} \right)
\]

We solved equation (27) for the contact and channel region, respectively, where the dimensionless fitting parameters \(\alpha_{contact} = 0.05\) and \(\alpha_{channel} = 0.18\) were used, respectively (see method section). Figure 3 shows the band shift as a function of the applied gate-source voltage \(V_{GS}\) in the center of the channel (solid blue line) and the contact region (dashed yellow line). Despite an applied voltage of \(\pm 20\) V, the band shift in the contact region is only about \(\pm 0.5\) eV, which can be explained by the fact that graphene is a semi-metal whose density of states is zero only at the Dirac point. Upon applying a gate voltage, the energy levels are shifted w.r.t. the Fermi level, and the screening mechanism by the quantum capacitance comes into effect immediately. The behavior of the band shift in the center of the channel, on the other hand, shows a nearly linear \(V_{GS}\) dependence at \(V_{GS} = 0\) because the Fermi level is within the bandgap of the CNT where the quantum capacitance is zero. If \(V_{GS}\) is increased (decreased), a cusp occurs after crossing the first van Hove singularity, and we
Fig. 2 The spectral function of the carbon nanotube at varying carbon nanotube/graphene spacing. The interaction strength between the graphene electrode and the carbon nanotube (CNT) on top is related to the broadening of the peaks in the spectral function \( A(E, k_z) \): strong interactions cause smearing of \( A(E, k_z) \). The spectral function is plotted in a 2D-heatmap plot over the energy \( E \) (with respect to the Fermi level \( E_F \)) and the wavevector \( k_z \). a At a spacing of \( d_{gr/CNT} = 5.0 \, \text{Å} \), the peaks are sharp and distinct. Smaller spacings lead to a smearing of the peaks, although the key features (bands and bandgap) are still visible (b and c). d At a spacing of 3.0 \, \text{Å}, some bands overlap while the semiconducting property of the CNT remains. This indicates that graphene electrodes do not destroy the semiconducting property of the CNT by metalizing it, as reported for Ni or Ti contacts27. The scale bar shows the logarithmic spectral function \( \log A(E, k_z) \) normalized to the range of values between 0 and 1.

Fig. 3 Gate efficiency in the center of the channel and the contact region. The gate induced shift of the energy bands \( \xi \) in the channel center (solid blue line) and the contact region (dashed yellow line) as a function of the gate-source voltage \( V_{GS} \). Compared to metallic electrodes, the graphene electrodes cannot entirely screen the carbon nanotube (CNT) from the gate field, whereby the CNT can also be electrostatically doped in the contact region. We explain the almost linear behavior of the band shift in the channel center by the fact that the Fermi level lies within the bandgap of the CNT, where the quantum capacitance is zero. For slightly increased (decreased) gate-source voltages, the linear behavior is damped rapidly because the Fermi level reaches the first van Hove singularity (VHS). We observe a strongly nonlinear response. The cusps, which originate from the van-Hove singularities, are annotated by the red markers in Fig. 3. In the contact region, we do not see any linear behavior. This is because graphene is a semi-metal and the partial screening of the CNT occurs even at small voltages.

Band diagram from the first principles. We obtain insights into the quantum transport in CNTFETs with graphene electrodes by extracting the band diagram along the CNT axis, i.e., the \( z \)-dependence of the valence and conduction band edges, \( E_V \) and \( E_C \). Eq. (37), respectively. These were plotted together with another \( z \)-dependent quantity, the local density of states \( D(E, z) \) Eq. (24), shown as a logarithmic color map (Fig. 4). The simulated atomistic system has a channel length of \( L_{contact} = 17 \, \text{nm} \) and semi-infinite contacts (\( L_{channel} = \infty \)). The geometry file for the CNT/graphene system used in this simulation can be found in Supplementary Data 2. Figure 4a shows \( E_V, E_C, \) and \( D(E, z) \) at zero bias \(( V_{DS} = 0, V_{GS} = 0) \). The simulated bandgap of the carbon nanotube is 0.816 eV, which is close to the experimental value for (9,8) carbon nanotubes (0.879 eV)42. The Fermi level in the channel region is 0.155 eV below the center of the bandgap and slightly higher at the contact region, indicating a weak p-doping of the CNT. This weak p-doping is a consequence of the similar work functions of the graphene and the carbon nanotube. We observe an almost flat band diagram along the \( z \)-axis because the hole inflow from the graphene to the tube is small. Ambipolar Schottky barriers for electrons and holes (defined as \( E_C - E_F \) and \( E_F - E_V \), respectively) can be observed at the contact/channel interfaces (white vertical lines). Analogous to Fig. 4a, in Fig. 4b, we show the unbiased band diagram for CNTFETs with Pd contacts. In contrast to the flat bands in gr/CNT contacts, CNTs in contact with Pd show strong doping which results from the large work function difference. The Fermi level in the contact regions falls several hundred eV below the valence band edge, resulting in a strong band bending and Ohmic contacts for holes (see Fig. 4b)24. Fig. 4c, d show the band bending of the devices with graphene contacts at a constant drain-source voltage \( V_{DS} = -0.5 \, \text{V} \) and a gate-source voltage of \( V_{GS} = 20 \, \text{V} \) and \( V_{GS} = -20 \, \text{V} \), respectively. As discussed in the previous
The on-state conductivity is plotted against the carbon nanotube/graphene spacing $d_{\text{gr/CNT}}$ on a logarithmic scale. The applied bias is $V_{\text{DS}} = -0.5$ V and $V_{\text{GS}} = -20$ V. We observe a strong dependence on $d_{\text{gr/CNT}}$ for devices with finite contact lengths ($L_{\text{contact}} = 50$ nm blue and $L_{\text{contact}} = 200$ nm yellow). The on-state conductivity of devices with infinite contact length (green) does not depend on the CNT/graphene spacing. We explain this by a saturation of the charge inflow from the electrodes. To improve the on-state conductivity, either the contact spacing must be reduced by purifying the CNT from residual polymers, or the contact length has to be increased by depositing longer CNTs. With infinite contact length, the conductivity reaches a theoretical limit of 0.6$G_0$.

**Conductivity scaling with the contact length and CNT/graphene spacing.** To understand the effect of the contact length $L_{\text{contact}}$ and graphene/CNT spacing $d_{\text{gr/CNT}}$ on the performance of the all-carbon FET and to derive design rules for high-efficient devices, we extracted the on-state conductivity for systems with finite contact lengths $L_{\text{contact}} = [50 \text{ nm}, 200 \text{ nm}, \infty]$. The on-state conductivity is defined as $G \equiv I_{\text{on}}/V_{\text{DS}}$, where we obtain the on-state current $I_{\text{on}} \equiv I_{\text{DS}}( -20 \text{ V}, -0.5 \text{ V})$ with the Landauer equation (38). The transmission functions $T(E)$ at different gr/CNT spacings are shown in supplementary figures 3, 4, and 5. Figure 5 shows the scaling of the on-state conductivity $G$ with the gr/CNT spacing $d_{\text{gr/CNT}}$. For devices with contact lengths of 50 nm and 200 nm, we observe a significant decrease in the on-state conductivity with increasing contact spacing $d_{\text{gr/CNT}}$. For a contact spacing of 3.0 Å, the conductivity is 0.1$G_0$ for $L_{\text{contact}} = 50$ nm and 0.5$G_0$ for 200 nm contact length. The conductivity at infinite contact length is 0.6$G_0$, regardless of the contact spacing. In summary, we observe that the charge transport between the graphene electrodes and the CNT strongly depends on the contact spacing $d_{\text{gr/CNT}}$ (see Fig. 2). Therefore, contact spacing is the limiting factor in the simulated devices with finite contact length.
For devices with infinite contact lengths, the contact spacing is irrelevant for the conductivity since the charge in flow in the contact region is saturated in any case. Our results imply that high on-state currents in all-carbon FETs can be achieved by either reducing the contact spacing (by removing the polymer residues around the CNT) or employing longer CNTs to increase the contact length.

Experimental verification. As already discussed, the experimental devices and their virtual twins display similarities regarding their architecture, especially in the case of the single CNT channel. Hence, we compare the measured IV characteristics with the simulations to verify the model. The electrical characterization of the experimental devices was performed at different temperatures and with gate-source voltages ranging from $-20$ V to 20 V. We estimate a channel length of 100 nm for the experimental devices by measuring the distance between source- and drain electrodes in the scanning electron micrograph (Fig. 1b). Since the contrast between the graphene electrodes and the CNT is too weak for the SEM method, we could not measure the contact length. In the theoretical part of this work, we simulated quantum transport through the atomistic structure (Fig. 1d) with a 50 nm contact length and a channel length of 18.4 nm. The channel length was taken to be smaller than in the experiment to reduce computational costs. We regard the CNT channel as a potential barrier with finite height and length, where the length primarily plays a role in so-called interband tunneling processes. The longer the channel, the more the tunneling processes are suppressed. For 100 nm long channels, we assume that no tunneling currents occur, whereas they do so in devices with short channel lengths. By suppressing the transmission coefficient within the energy regimes, corresponding to interband tunneling, we justify the simulation of 18.4 nm channel devices and compare the results with experimental devices with 100 nm channel lengths (see the Method section for more details). Due to the surface roughness of the SiO$_2$ substrate, the uneven graphene electrodes, and the remaining polymer wrapped around the CNT and it is not feasible experimentally to control or measure the CNT/graphene spacing. Therefore, we investigated the temperature and $V_{DS}$ dependence of the fabricated devices and the simulation model to broaden the parameter space for experimental verification. We calculate the current using the Landauer formula (38) and compare the experimental with the simulated currents for the following aspects: On-state currents and the off-state interval.

Figure 6a shows the experimental currents of devices D1 and D2 at different temperatures $T = [4 \text{ K}, 25 \text{ K}, 100 \text{ K}, 150 \text{ K}]$ and fixed drain-source voltage $V_{DS} = -0.9$ V. For $T < 150 \text{ K}$, the off-state regime for D1 is between $-5$ V and 10 V, whereas the off-state regime of D2 ranges between 0 V and 10 V. The difference in off-state regimes between D1 and D2 can be due to a variety of reasons, including trap states in the channel region. The p-branch on-state current ($V_{GS} = -20$ V) of D1 agrees well with the current of D2. However, the n-branch currents ($V_{GS} = 20$ V)
differ significantly between D1 and D2. For the simulated currents at different temperatures (see Fig. 6b), the off-state regime ranges from approximately $-2.0 \, \text{V}$ to $10 \, \text{V}$ to $15 \, \text{V}$, depending on the temperature. Particularly noteworthy is the fact that simulated p-state currents agree well with the measured ones. The simulated n-branch currents differ from all experiments, whereas the experiments differ from each other as well. To find the reason for the strong n-branch discrepancy, further experimental studies are needed. We suspect that trap-states in the oxide layer cause immobilization of the electrons which leads to strong differences in the n-branch. The variability of the IV characteristics is discussed in e.g. Franklin et al.\textsuperscript{50}. Overall, the temperature-induced variations of the simulated currents are less pronounced than the variations in the experiments. The $V_{DS}$ dependence at constant temperature ($T = 4 \, \text{K}$) of D1 and D2 are shown in Fig. 6c. We observe similar off-state regimes and p-branch on currents as presented in Fig. 6a. But the variations in the currents of the n-branch increased greatly. The simulation results at constant temperature ($T = 4 \, \text{K}$) and varying drain-source voltage $V_{DS}$ are shown in Fig. 6d. Again, p-polar on-state currents and off-regime seem to be consistent but as mentioned above further investigations into the n-branch currents need to be done. In general, we consider our model to be capable of predicting p-currents and the off-state regimes for all-carbon FETs.

**Conclusion**

Previous works\textsuperscript{51–55} have investigated CNT/graphene hybrid structures and advocated them for future electronic devices. However, there is still a lack of knowledge about the parameters which critically affect the efficiency of such structures and how they can be systematically improved. Here, we have developed an ab-initio based model of quantum transport in all-carbon transistors, capable of simulating all-carbon atomistic structures with arbitrary contact lengths and graphene-CNT spacing. By using both experimental and simulation data we have discovered the following properties of this device: (a) at zero bias, the all-carbon transistor is an ambipolar electronic device with Schottky barriers for electrons and holes at the contact/channel interfaces; (b) in stark contrast to CNTFETs with metallic contacts, the electric field from the bottom gate is only partially screened by the graphene electrodes, so – in addition to the channel region – the CNT in the contact region can also be electrostatically doped to turn the Schottky contacts to Ohmic contacts for electrons ($V_{GS} > 0$) or holes ($V_{GS} < 0$); (c) the conductivity of the all-carbon transistor can be increased up to almost $G_0$ by either purifying the

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**Fig. 7 Schematic overview of the procedure to calculate the graphene self-energy and the following decoration of the carbon nanotube (CNT) contact elements.**

**a** Module 1 represents the carbon system of the all-carbon field effect transistor deep within the contact region and is visualized as a 3D block tight-binding system with the red and blue spheres representing the CNT and graphene unit cells, respectively. The reference unit cells for the $k_z$-space transformations are denoted with $R_0$ (CNT) and $r_0$ (graphene).

**b** After $k_z$-transformation, one obtains a planar block tight-binding system where the $k_z$-dependent CNT element is depicted in purple, while the graphene on-site cells are green.

**c** Decimation of the semi-infinite chain results in a finite planar system with an additional energy dependence from which the graphene self-energy in $k_z$ – space can be computed.

**d** Inverse Fourier transformation is used to obtain the on-site $\sigma_0(E)$ and hopping $\sigma_t(E)$ elements of the self-energy.

**e** Visualization of module 2 as an effective one-dimensional tight-binding chain. All matrix elements relevant for quantum transport calculations of CNTFETs with arbitrary contact lengths are extracted from the finite matrices $H^{(2)}$ and $S^{(2)}$. In accordance with the usual non-equilibrium Greens function scheme, the left $H_L$, central $H_C$, and right $H_R$ subsystems are specified. On- and off-site hopping matrices in the contact regions are decorated with the self-energies, which have been obtained from module 1.
CNTs to reduce the contact spacing or by increasing the contact length; (d) we attributed the low p-branch on currents in the experimental devices to residual polymers wrapped around carbon nanotubes. Our developed and verified method allows us to simulate quantum transport for systems with realistic geometries at the quantum-mechanical level and thus paves the way for a rational design of all-carbon electronic devices. The immediate practical implication of our work is this: To increase the on-state current in all-carbon transistors, either increasing the contact length, or removing the residual polymer is necessary.

Methods

CNT Synthesis. SWCNTs enriched with (9,8) nanotubes were synthesized using Co/SiO2 catalysts by chemical vapour deposition. SEM images of the catalysts before and after SWCNT synthesis are shown in supplementary figure 1. Following the previously published methods,56–58 Co/SiO2/Si catalysts with 1 wt% Co were prepared by incipient wetness impregnation using Co (II) sulfate hexahydrate (CoSO4·7H2O, Sigma-Aldrich) and fumed silica (SiO2, Cab-O-Sil M-5, Sigma-Aldrich). During SWCNT growth, metal precursor was loaded in a quartz tube and the temperature was first reduced in pure H2 (1 bar, 99.99%) from room temperature to 540 °C. Then the temperature was increased to 780 °C under Ar (99.99%). At 780 °C, catalysts were exposed to pressured CO (6 bar, 99.99%) with a flow rate of 200 sccm for 1 h. CO was purifed by a purifier (Nanochem, Matheson Gas Products) before entering the reactor to remove carbonyl residues. As-synthesized SWCNTs were isolated using a 1.5 M NaOH aqueous solution for 2 hours and then centrifuged to dissolve SiO2. Afterwards, carbon materials filtered on a nylon membrane were used for further purifcation and enrichment. The Raman spectrum of as-synthesized SWCNTs deposited on catalysts and UV-vis-NIR spectrum of the SWCNT suspension are shown in supplementary figure 2.

Device fabrication and characterization. P-doped silicon wafer with 300 nm thermal oxide (Active Business Company, resistance Ω <0.005 cm) was used as substrate and diced into 10 × 10 mm2 samples. In three lithography steps tungsten gate electrodes for 5 min, leading to bridging graphene electrodes by individual CNTs. Afterwards the sample was rinsed with toluene and annealed for 1.5 h at 780 °C. The graphene on- and off-site matrices with

$$H_{\text{CNT}}(k_z) = \sum_{\text{neig}-1} \sum_{\text{1D-2D contacts}} \text{H}^{(1)}[R_c; r_e, n_z, n_x, \text{d}^z_{\text{CNT}}]$$

(1)

with $n_z (2)$ and $n_x (3)$ CNTs are in detail elsewhere.49,50 Integration of CNTs between graphene electrodes was performed using ac-dielectrophoresis.41 The suspension was diluted in toluene (1:10) and a 10 µl droplet was placed over the sample. Using an Agilent 33220A function generator, an alternating voltage (0.5 V, 100 kHz) was applied between common and gate electrodes for 5 min. The overlap matrix $\text{SO}_{17}$ and the Hamiltonian $H_{17}$ can be visualized by the block tight-binding scheme shown in Fig. 7. The red and blue beads represent the on-site matrices of graphene and the CNT, respectively. The inter-block interactions are not explicitly displayed. Using the translation symmetry, we perform a Fourier transformation from $z \rightarrow k_z$ space.49,50 and obtain $N_{k_z}$ planar block tight-binding systems shown in Fig. 7b, where $N_{k_z}$ is the number of $k_z$-sampling points and $k_z \in [-\pi/d_{k_z}; \pi/d_{k_z}]$. The $k_z$-dependent on- and off-site matrices are obtained by:

$$t_{n_x}(k_z) = \sum_{\text{neig}-1} \text{H}^{(1)}[R_c; r_e, n_z, n_x, \text{d}^z_{\text{CNT}}]$$

(2)

$$a_{n_k}(k_z) = \sum_{\text{neig}-1} \text{H}^{(1)}[t_0 + \text{d}^z_{\text{CNT}}; n_z, \text{d}^z_{\text{CNT}}]$$

(3)

where $R_c$ denotes the center of mass position of the CNT unit cell in the center of module $1$ and $r_e$ the graphene unit cell beneath. $H^{(1)}[v, u]$ indicates the interaction between the unit cells at position $v$ and $u$ (on-site element for $v = u$) and $n_z$ stands for the $z$-coordinate. The CNT block $H_{n_z}(k_z)$ is represented in the basis of atomic orbitals by an $N \times N$ matrix for each sampling point in momentum-space. The graphene on- and off-site elements ($a_{n_k}(k_z)$ and $\beta_{n_k}(k_z)$) form $M \times M$ matrices, so the coupling matrices between the CNT and graphene subsystems ($t_{n_x}(k_z)$) are $N \times M$ matrices. The overlap matrices in $k_z$ space are obtained by replacing $H^{(1)}$ with $S(\theta)$ in equations (1)-(4). The graphene on- and off-site matrices with $|n_z| > 2$ are replaced by $a_{n_k}(k_z)$ and $\beta_{n_k}(k_z)$ respectively, since the influence of the CNT on these and any further elements can be neglected. The resulting tight-binding system is composed of two semi-infinite block tight-binding chains on the left $H_{\text{left}}^{(1)}$ and right $H_{\text{right}}^{(1)}$ and a finite two-dimensional system in between (see Fig. 7b). The Hamiltonian of the semi-
The Hamiltonian and the overlap matrix corresponding to the channel are given by:

\[ H_{\text{con}} = \sum_{i=1}^{N_{\text{contact}}} \sum_{j=1}^{N_{\text{contact}}} h_{ij} \langle \phi_{\text{con},i} | \phi_{\text{con},j} \rangle \]

\[ S_{\text{con}} = \sum_{i=1}^{N_{\text{contact}}} \sum_{j=1}^{N_{\text{contact}}} s_{ij} \langle \phi_{\text{con},i} | \phi_{\text{con},j} \rangle \]

(14)

(15)

With the introduced elements of \( H_{\text{con}} \) and \( S_{\text{con}} \), it is possible to simulate CNTTFETs with arbitrary contact lengths. Therefore it is assumed that the matrices further within the contact regions do not differ from \( H_{\text{con}} \) and \( S_{\text{con}} \). The contact length needs to be chosen in units of the unit cell size \( d_{\text{contact}} = d \cdot N_{\text{contact}} \). With \( N_{\text{contact}} = 1, 2, \ldots \)

The decorated contacts are iteratively decimated using the Green’s function:

\[ G^{(i)}(E) = \left[ \begin{array}{c|c} \hat{E}^{\text{con}}_n - H(E) \end{array} \right]^{-1} \]

(16)

(17)

(18)

The iterative procedure is conducted until all contact elements have been decimated to compute the final self-energies with the obtained surface Green’s functions \( G^{(i)}(E) \) and \( G^{(i)}(E) \), which converge to the exact Green’s functions.

\[ \Sigma_{\text{L}} = \left[ \begin{array}{c|c} \hat{E}^{\text{LS}}_n - V_{\text{LS}} \end{array} \right] G^{(i)}(E) \left[ \begin{array}{c|c} \hat{E}^{\text{LS}}_n - V_{\text{LS}} \end{array} \right]^{-1} \]

\[ \Sigma_{\text{R}} = \left[ \begin{array}{c|c} \hat{E}^{\text{SR}}_n - V_{\text{SR}} \end{array} \right] G^{(i)}(E) \left[ \begin{array}{c|c} \hat{E}^{\text{SR}}_n - V_{\text{SR}} \end{array} \right]^{-1} \]

(19)

(20)

For infinitely long contacts, the highly convergent method\(^{69,70}\) used earlier is used to obtain the surface Greens functions.

The last step is to decorate the matrices that belong to the left and right end of the channel region with the self-energies:

\[ H_{\text{con}} = \sum_{i=1}^{N_{\text{contact}}} \left[ \begin{array}{c} h_{i1} + \Sigma_{\text{L}}^{(i)}(E) \end{array} \right] \left[ \begin{array}{c} h_{i1} + \Sigma_{\text{L}}^{(i)}(E) \end{array} \right]^{-1} \]

\[ S_{\text{con}} = \sum_{i=1}^{N_{\text{contact}}} \left[ \begin{array}{c} s_{i1} + \Sigma_{\text{L}}^{(i)}(E) \end{array} \right] \left[ \begin{array}{c} s_{i1} + \Sigma_{\text{L}}^{(i)}(E) \end{array} \right]^{-1} \]

(21)

The original system consisting of 1D (CNT) and 2D (graphene) components was reduced to an effective quasi-1D system with energy dependence using the modular approach. The method was developed based on the CNT/graphene contact as an exemplary system but can effortlessly be applied to various 1D/2D extended contacts.

To calculate the local density \( D(E, i) \), and transmission coefficient \( T(E) \), the retarded Green’s function of the decorated channel system is required:

\[ G_{\text{C}}(E) = \left[ \begin{array}{c} \hat{E}^{\text{con}}_n - H(E) \end{array} \right]^{-1} \]

(22)

Depending on the channel length, it is numerically costly to determine \( G_{\text{C}} \), with equation (22), hence the recursive algorithm suggested by Klimeck\(^{59}\) is used to obtain the relevant elements of the Green’s function, namely, \( G_{\text{C},1,1} \), \( G_{\text{C},2,1} \), \( G_{\text{C},2,2} \), and \( G_{\text{C},3,1} \), where \( G_{\text{C},i,j} \) is an \( N \times N \) matrix and the \( a, b \) element of the block-matrix \( G_{\text{C},i,j} \).

Afterward, the transmission coefficient and density of states can be found:

\[ T(E) = \text{Tr} \left[ G_{\text{C},1,1} G_{\text{R}} G_{\text{G},1,1} \right] \]

\[ D(E, i) = \sum_{j=1}^{N_{\text{contact}}} \left( \text{Tr} \left[ G_{\text{C},i,j} S_{\text{L}} \right] + \text{Tr} \left[ G_{\text{C},i,j} G_{\text{C},j,l} S_{\text{L}} \right] \right) \]

\[ \text{Tr} \left[ G_{\text{C},i,j} S_{\text{L}} \right] \text{ for } i = 1 \]

\[ \text{Tr} \left[ G_{\text{C},i,j} G_{\text{C},j,l} S_{\text{L}} \right] \text{ for } i < j \]

\[ \text{Tr} \left[ G_{\text{C},i,j} S_{\text{L}} \right] \text{ for } i = j \]

\[ \text{Tr} \left[ G_{\text{C},i,j} G_{\text{C},j,l} S_{\text{L}} \right] \text{ for } i = 1 \]

where \( \Gamma_{\text{L}}(R) = \left( \begin{array}{c} \Sigma_{\text{L}}(R) - \Sigma_{\text{L}}(R) \end{array} \right) \) is related to the rates of elastic electron scattering from the electrodes to the channel region and the other way round.

Electrode model: For the drain and gate-source electrodes, an idealized model was used (Fig. 1c). Highly doped silicon served as the gate electrode, followed by 300 nm SiO2 as an insulator layer. The graphene sheets were used as source and drain electrodes. In the model, the source electrode is grounded and the voltages
are defined as:

\[ V_{GS} = \phi_G - \phi_S \]  \hspace{1cm} (25)
\[ V_{DS} = \phi_P - \phi_S \]  \hspace{1cm} (26)

where \( \phi_{QGOS} \) is the electrostatic potential at the gate- (drain-) electrode. Unlike metallic electrodes, it is assumed that gate-voltage-induced doping of the CNT occurs not only in the channel but also in the contact regions since graphene is semi-metallic. The electrically driven shift \( \xi \) of the CNT band structure is described by\(^{72}\):

\[ \frac{\partial \xi}{\partial(-eV_{GS})} = \frac{1}{1 + \alpha \frac{\sqrt{V_{GS}}}{\xi}} \]  \hspace{1cm} (27)

where \( C_i = \varepsilon_\text{G} / L \) denotes the classical capacitance of the insulating layer (\( \varepsilon_\text{G} = 3.9 \)) with thickness \( L \), \( \alpha \) is a dimensionless parameter and \( C_0(V_{GS}) \) stands for the quantum capacitance, defined as:

\[ C_0(V_{GS}) = e^2 \int D(E) \left( \frac{\partial f(E - eV_{GS})}{\partial E} \right) dE. \]  \hspace{1cm} (28)

Eq. (27) is solved separately for both the contact region and the channel where \( \delta_{\text{contact}} = 0.05 \) for the contact and \( \delta_{\text{channel}} = 0.18 \) for the channel yielded results that most closely matched the experiment. The “CNT on graphene” is deemed to have two quantum capacitances in a parallel circuit, yielding a total quantum capacitance in the contacts:

\[ C_Q = C_{Q,\text{cm}} + C_{Q,\text{gr}}. \]  \hspace{1cm} (29)

in which, the quantum capacitance of the CNT is calculated with equation (28). For the graphene part, an analytic expression\(^{52}\):

\[ C_{Q,\text{gr}}(V_{GS}) = \frac{2}{\pi} \left( \frac{e}{k_B T} \right) \kappa B T \left( 2 + 2 \cosh \left( \frac{eV_{GS}}{k_B T} \right) \right). \]  \hspace{1cm} (30)

was used, where \( \kappa = 10^3 \text{cm/s} \) is the typical Fermi-velocity in graphene. The band shift along the channel is determined by the empiric formula\(^{36,27}\):

\[ \xi_{\text{channel}}(eV_{GS}, V_{DS}) = \xi_{\text{contact}} - \xi_{\text{center}} e^{-\frac{eV_{GS}}{k_B T}} + \xi_{\text{center}} - \xi_{\text{contact}} e^{-\frac{eV_{DS}}{k_B T}}, \]  \hspace{1cm} (31)

with the right (left) end position of the channel \( \xi_{\text{G}}(a,b) \) the decay length, and the CNT diameter \( d_{\text{CNT}} \). Again, equation (27) is used to find the band shift in the center of the CNT section.

**Combined electrode model and modular approach.** To rigorously incorporate the electrostatics into the quantum transport calculation, the Kohn-Sham equations need to be solved self-consistently for each \( V_{GS}, V_{DS} \)-configuration. With the electrode model at hand, one is capable of calculating a realistic response of the carbon system to externally applied fields, which is then combined with the modular DFT+NEGF approach to compute a voltage-dependent transmission coefficient. Therefore, the matrices in equation (13) need to be adapted according to:

\[ H_{E}\left(E, V_{GS}\right) = H_{L}(E) + \xi_{\text{contact}}(V_{GS}) S_{L} \]  \hspace{1cm} (32)
\[ H_{R}(E, V_{GS}, V_{DS}) = H_{R}(E) + \xi_{\text{contact}}(V_{GS}) - eV_{DS} S_{R} \]  \hspace{1cm} (33)

which results in voltage dependence of the self-energies \( \Sigma_{E}(E, V_{GS}) \) and \( \Sigma_{E}(E, V_{GS}, V_{DS}) \), following the same logic, each element in the decorated channel Hamiltonian (14) is modified individually:

\[ H_{E}\left(E, V_{GS}, V_{DS}\right) = \left[ H_{L} + \xi_{\text{channel}}(E) S_{L} \right] I_{\{1,1\}} + \sum I_{\{1,1\}} + \sum I_{\{1,1\}} \right] I_{\{1,1\}} \right] I_{\{1,1\}} \right] \]  \hspace{1cm} (34)

Again, the corresponding block elements of Green’s function will be extracted using recursive method\(^{33}\) and the transmission coefficient \( T(E, V_{GS}, V_{DS}) \) is obtained using equation (23).

**Suppression of the interband tunneling.** The choice of the channel length \( n \) is a trade-off between a realistic representation of the manufactured CNTFETs (\( L_{\text{channel}} = 100 \text{ nm} \)) and the computing time required to simulate quantum transport through systems with long channel lengths. In the used model, the impact of channel length is primarily relevant to interband tunneling processes which are promoted by short channels. Therefore, quantum transport was simulated for short channel systems by suppressing interband tunneling for this purpose, the band bending along the symmetry axis of the CNT needs to be determined and the energy range between the maximum of the conduction band edge and the minimum of the valence band edge is excluded. The conduction and valence band at point \( \pm \frac{1}{2} \) \( d_{n} \) is computed by the following steps: First, the corresponding, biased on- and off-site Hamiltonian and overlap matrices are extracted for the site \( i \) and the on-site matrices in momentum space at \( k_{\text{f}} = 0 \) are computed:

\[ \psi_{\text{f}}(k_{0} = 0) = H_{X_{i=1}}^{0} + H_{X_{i=1}}^{0} + H_{X_{i=1}}^{0} \]  \hspace{1cm} (35)
\[ \psi_{\text{f}}(k_{0} = 0) = S_{X_{i=1}}^{0} + S_{X_{i=1}}^{0} + S_{X_{i=1}}^{0} \]  \hspace{1cm} (36)

where \( X = \{L, S, R\} \) stand for the above-defined regions of the entire Hamiltonian. For the sake of simplicity, the selfenergies \( \Sigma_{L, S, R} \) and \( \delta_{L, S, R} \) were neglected in the following steps.

Secondly, the general eigenvalue problem

\[ \psi_{L}^{(i)} = \xi_{L}^{(i)} \psi_{L}^{(i)} \]  \hspace{1cm} (37)

where \( \mu \) denotes the band-index, is solved using the eig method implemented in the scipy library. The \( N \) obtained eigenvalues correspond to the electronic bands of the CNT unit cell at position \( \xi \). The valence and conduction band edges are given by \( E_{V,i} = E_{F,i}^{\text{NS}} = E_{V,i}^{\text{NS}} = E_{F,i}^{\text{NS}} \) for \( N_{E} = 10001 \) sampling points on the energy axis, we chose a \( 0 \) of 40 sampling points.

Finally, the current at a given gate- and drain-source voltage is computed with the Landauer formula\(^{52}\):

\[ I_{\text{DS}}(V_{GS}, V_{DS}) = e \int T(E, V_{GS}, V_{DS})(f(\epsilon) - f_{0}(E - eV_{DS})) dE. \]  \hspace{1cm} (38)

**Data availability**

The data that support the findings of this study are available in the paper and its supplementary information files, or from the corresponding author upon reasonable request. The geometry file and cp2k input files for modules 1 and 2 can be found in Supplementary Data 1 and Supplementary Data 2, respectively.

**Code availability**

The python code used for the numerical simulations discussed in this paper is available from the corresponding authors upon reasonable request. For the DFT calculations, the software package cp2k (version 5.1) was used.

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**References**

1. Avouris, P., Chen, Z. & Perebeinos, V. Carbon-based electronics. Nat. Nanotechnol. 2, 665–615 (2007).
2. Venema, L. Silicon electronics and beyond. Nature 479, 309 (2011).
3. Artękowicz, E., Kaempgen, M., Hecht, D. S., Roth, S. & Grüner, G. Transparent and flexible carbon nanotube transistors. Nano Lett. 5, 757–760 (2005).
4. Aikawa, S. et al. Deformable transparent all-carbon-nanotube transistors. Appl. Phys. Lett. 100, 063502 (2012).
5. Eda, G., Fanchini, G. & Chhowalla, M. Large-scale ultrathin films of reduced graphene oxide as a transparent and flexible electronic material. Nat. Nanotechnol. 3, 270–274 (2008).
6. Jang, S. et al. Flexible, transparent single-walled carbon nanotube transistors with graphene electrodes. Nanotechnology 21, 425201 (2010).
7. Charlton, J.-C., Blase, X. & Roche, S. Electronic and transport properties of nanotubes. Rev. Mod. Phys. 79, 677–732 (2007).
8. Ding, J. W., Van, X. H. & Cao, J. X. Analytical relation of band gaps to both chirality and diameter of single-wall carbon nanotubes. Phys. Rev. B 66, 073401 (2002).
9. Sukor, G. et al. Structural dependence of excitonic optical transitions and band-gap energies in carbon nanotubes. Nano Lett. 5, 2314–2318 (2005).
10. Sukor, S. et al. Diameter-dependent band gap modification of single-walled carbon nanotubes by encapsulated fullerene. J. Phys. Chem. C. 113, 571–575 (2009).
11. Avouris, P. Molecular electronics with carbon nanotubes. Acc. Chem. Res. 35, 1026–1034 (2002).
12. Xiao, M. et al. n-type Dirac-source field-effect transistors based on a graphene/ carbon nanotube heterojunction. Adv. Electron. Mater. 6, 2000258 (2020).
13. Tuleskis, G. S. et al. Toward high-performance digital logic technology with carbon nanotubes. ACS Nano 8, 8730–8745 (2014).
14. Byrne, M. T. & Gun’ko, Y. K. Recent advances in research on carbon nanotube–polymer composites. Adv. Mater. 22, 1672–1688 (2010).
15. Allen, B. L., Khiambarde, P. D. & Star, A. Carbon nanotube field-effect transistor-based filters. Adv. Mater. 19, 1439–1451 (2007).
16. Macdonald, R. A., Laurenzi, B. F., Viswanathan, G., Ajayan, P. M. & Stegeman, J. P. Collagen–carbon nanotube composite materials as scaffolds in tissue engineering. J. Biomed. Mater. Res. Part A 74A, 489–496 (2005).
17. Pyatkov, F. et al. Cavity-enhanced light emission from electrically driven carbon nanotubes. Nano Lett. 14, 984–989 (2014).
18. Khasminskaya, S. et al. Fully integrated quantum photonic circuit with an electrically driven light source. Nat. Photonics 8, 737–742 (2016).
19. Pyatkov, F. et al. Toward high-performance digital logic technology with carbon nanotubes. ACS Nano 8, 8730–8745 (2014).
20. Byrne, M. T. & Gun’ko, Y. K. Recent advances in research on carbon nanotube–polymer composites. Adv. Mater. 22, 1672–1688 (2010).
21. Allen, B. L., Khiambarde, P. D. & Star, A. Carbon nanotube field-effect transistor-based filters. Adv. Mater. 19, 1439–1451 (2007).
22. Macdonald, R. A., Laurenzi, B. F., Viswanathan, G., Ajayan, P. M. & Stegeman, J. P. Collagen–carbon nanotube composite materials as scaffolds in tissue engineering. J. Biomed. Mater. Res. Part A 74A, 489–496 (2005).
23. Pyatkov, F. et al. Cavity-enhanced light emission from electrically driven carbon nanotubes. Nano Lett. 14, 984–989 (2014).
24. Khasminskaya, S. et al. Fully integrated quantum photonic circuit with an electrically driven light source. Nat. Photonics 8, 737–742 (2016).
25. Pyatkov, F. et al. Toward high-performance digital logic technology with carbon nanotubes. ACS Nano 8, 8730–8745 (2014).
26. Byrne, M. T. & Gun’ko, Y. K. Recent advances in research on carbon nanotube–polymer composites. Adv. Mater. 22, 1672–1688 (2010).
27. Allen, B. L., Khiambarde, P. D. & Star, A. Carbon nanotube field-effect transistor-based filters. Adv. Mater. 19, 1439–1451 (2007).
28. Macdonald, R. A., Laurenzi, B. F., Viswanathan, G., Ajayan, P. M. & Stegeman, J. P. Collagen–carbon nanotube composite materials as scaffolds in tissue engineering. J. Biomed. Mater. Res. Part A 74A, 489–496 (2005).
29. Pyatkov, F. et al. Cavity-enhanced light emission from electrically driven carbon nanotubes. Nano Lett. 14, 984–989 (2014).
30. Khasminskaya, S. et al. Fully integrated quantum photonic circuit with an electrically driven light source. Nat. Photonics 8, 737–742 (2016).
31. Pyatkov, F. et al. Toward high-performance digital logic technology with carbon nanotubes. ACS Nano 8, 8730–8745 (2014).
32. Byrne, M. T. & Gun’ko, Y. K. Recent advances in research on carbon nanotube–polymer composites. Adv. Mater. 22, 1672–1688 (2010).
33. Allen, B. L., Khiambarde, P. D. & Star, A. Carbon nanotube field-effect transistor-based filters. Adv. Mater. 19, 1439–1451 (2007).
34. Macdonald, R. A., Laurenzi, B. F., Viswanathan, G., Ajayan, P. M. & Stegeman, J. P. Collagen–carbon nanotube composite materials as scaffolds in tissue engineering. J. Biomed. Mater. Res. Part A 74A, 489–496 (2005).
35. Pyatkov, F. et al. Cavity-enhanced light emission from electrically driven carbon nanotubes. Nano Lett. 14, 984–989 (2014).
36. Khasminskaya, S. et al. Fully integrated quantum photonic circuit with an electrically driven light source. Nat. Photonics 8, 737–742 (2016).
37. Pyatkov, F. et al. Toward high-performance digital logic technology with carbon nanotubes. ACS Nano 8, 8730–8745 (2014).
38. Byrne, M. T. & Gun’ko, Y. K. Recent advances in research on carbon nanotube–polymer composites. Adv. Mater. 22, 1672–1688 (2010).
39. Allen, B. L., Khiambarde, P. D. & Star, A. Carbon nanotube field-effect transistor-based filters. Adv. Mater. 19, 1439–1451 (2007).
40. Macdonald, R. A., Laurenzi, B. F., Viswanathan, G., Ajayan, P. M. & Stegeman, J. P. Collagen–carbon nanotube composite materials as scaffolds in tissue engineering. J. Biomed. Mater. Res. Part A 74A, 489–496 (2005).
41. Pyatkov, F. et al. Cavity-enhanced light emission from electrically driven carbon nanotubes. Nano Lett. 14, 984–989 (2014).
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Author contributions
A.F., A.O., and W.W. conceived and designed the simulation part of this project. A.F. and A.O., developed and employed the methodology to simulate carbon nanotube/graphene self-energies and the simulation of the current-voltage characteristics and did the simulations for relevant quantities presented in this work. The experiments were conceived and designed by R.K., A.F., and F.P. The nanotube raw material was provided by Y.C., purified and length fractionated by F.H. Devices were fabricated by P.B. and F.P. Low-temperature electrical measurements were performed by P.B. and F.P. All authors contributed to the preparation of the manuscript. A.O., A.F., W.W., and R.K. wrote the manuscript.

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