Multicontrol Over Graphene–Molecule Heterojunctions

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ABSTRACT: The vertical configuration is a powerful tool recently developed experimentally to investigate field effects in quasi two-dimensional systems. Prototype graphene-based vertical tunneling transistors can achieve an extraordinary control over current density utilizing gate voltages. In this work, we study theoretically vertical tunneling junctions that consist of a monolayer of photoswitchable aryl azobenzene molecules sandwiched between two sheets of graphene. Azobenzene molecules transform between trans and cis conformations upon photoexcitation, thus adding a second knob that enhances the control over physical properties of the junction. Using first-principles methods within the density functional framework, we perform simulations with the inclusion of field effects for both trans and cis configurations. We find that the interference of interface states resulting from molecule–graphene interactions at the Fermi energy introduces a dual-peak pattern in the transmission functions and dominates the transport properties of gate junctions, shedding new light on interfacial processes.

INTRODUCTION

In miniaturizing metal-oxide-semiconductor field-effect transistors to sub-5 nm size, one encounters severe challenges in preserving system performance and reliability, and one must rely on new physics emerging from nanoscale material systems to overcome this obstacle. The vertical integration of tunneling field-effect transistors (TFETs) based on the stacking of two-dimensional (2D) layered materials has been explored as an alternative transistor architecture in recent years. Vertical TFET stacking layers of graphene with 2D insulators and semiconductors, such as hexagonal boron nitride (h-BN) and transition metal dichalcogenides, have been demonstrated to exhibit extraordinary control of the tunneling current via gate voltages. Equally, if not more, important, the vertical configuration introduces a technique to approach fundamental physics processes at interfaces, an emergent area in materials, chemical, and condensed matter physics.

When the thickness of a system is of nanoscale, interfacial physics governs the electronic, magnetic, and transport properties. For instance, the h-BN $|$ graphene interface is electrostatically sharp, whereas the dielectric response of WS2 is greatly affected by interface with graphene. Interface physics is in general not limited to nanoscale materials; interfaces between two bulk systems or between a bulk material and vacuum or air can also trigger emergent phenomena. Examples include the two-dimensional electron gas at a LaAlO3 $|$ SrTiO3 interface and the protected surface states of the celebrated topological insulators. Nanostructured 2D systems, which have bulk 2D extent but are finite in the third dimension, provide unique opportunities for investigating and understanding interfacial processes.

The subject of this study is TFETs based on graphene and organic materials. Recent advances in fabricating hybrid nanoscale heterostructures have made it possible to incorporate organic molecules in the design of vertical TFETs. Covalent bonds between molecules and graphene can form via dediazonation. It was proposed that such bonds enhance the flexibility of graphene $|$ molecule $|$ graphene junctions. The gate-voltage-tunable transport through graphene $|$ molecule interfaces has been attributed to modulation of the Schottky barriers at the interface. Organic molecules offer the advantage over inorganic materials that their properties can be modified by substituting various ligands; in particular, photoswitchability can be incorporated by inserting azobenzene ligands that can switch between trans and cis conformations.

The trans conformation has an energy of about 0.6 eV lower than that of cis. An energy barrier of approximately 1.6 eV needs to be overcome during a trans-to-cis transition. In experiments, a trans-to-cis isomerization occurs upon photoexcitation by light with a wavelength of 365 nm and a cis-to-trans isomerization at 420 nm. The electronic, magnetic, and photoelectronic properties of molecules on graphene have been studied previously. In this work, we investigate theoretically the interface states at graphene $|$ azobenzene $(containing) |$ graphene nanojunctions and the emerging phenomena when the gate voltage is turned on. Combined with the optical control over the trans and cis forms of azobenzene molecules, we propose a multicontrol charge transport process and the underlying physical origin.

COMPUTATIONAL METHODS

Calculations were carried out using density functional theory (DFT). The geometries of graphene $|$ trans $|$ graphene (Gr $|$ trans $|$ Gr) and graphene $|$ cis $|$ graphene (Gr $|$ cis $|$ Gr), as...
shown in Figure 1a,b, were fully optimized using the VASP package. The nuclei and frozen core electrons were modeled with the projector augmented-wave method. The weak interactions between molecules and the top graphene layer were treated using the van der Waals density functional. Integrals over the first Brillouin zone were carried out on a regular mesh of $55 \times 55 \times 1$ $k$-points, and the plane-wave cutoff for wave function expansion was set to 500 eV. The residual force on every atom is smaller than 0.01 eV/Å after relaxation.

We studied transport properties using the DFT-based nonequilibrium Green’s function method, which is widely used for molecular junctions. Within the generalized gradient approximation parameterized by Perdew–Burke–Ernzerhof, the electronic structure and transport properties were calculated using the SIESTA package, based on Troullier–Martins norm-conserving pseudopotentials and a pseudatomic orbital basis set. The electrostatic interaction was treated by the effective screening medium (ESM) approach that solves the Hartree potential with nonperiodic boundary conditions, and we recently adopted the ESM method to simulate gate effects. Additional electrons (holes) were added to the Gr | molecule | Gr system to simulate the positive (negative) gate voltage. An areal electron density of $6.24 \times 10^{12}$ cm$^{-2}$ corresponds to a gate electric displacement field of $\epsilon_0 E_g = 0.01$ C/m$^2$. Compared with the gate voltage and gate electric field ($E_g$), the electric displacement field, $\epsilon_0 E_g$, is a more convenient quantity because it is independent of the thickness or the dielectric constant of the dielectric material separating the Gr | molecule | Gr system and the gate electrode.

The molecule–graphene heterogeneous TFET is schematically shown in Figure 1. Azobenzene-containing molecules 4-(10-((4-(trifluoromethyl)phenyl)diazene)phenyloxy)benzene are anchored at the bottom graphene layer by a C–C bond, and the contact with the top graphene layer is of van der Waals nature. The leftmost and rightmost graphene regions serve as source and drain, respectively.

The curved part of the left graphene sheet follows the description in ref 43 where it was shown that electrons encounter little scattering. This configuration mimics the experimental configuration, and gate voltages are guaranteed to induce the same potential shift on source and drain. Equilibrium Green’s function and transmission probability were calculated from the Hamiltonian using a well-established procedure.
RESULTS

Transmission of Gr | molecule | Gr junctions depends on the conformation (trans and cis) of the molecule and can be modulated by the gate voltage, as shown in Figure 2. The Gr | trans | Gr junction has a transmission almost symmetric with respect to the negative and positive gate voltages, whereas transmission of the Gr | cis | Gr junction is much enhanced by positive gate voltages. With no gate voltage, the different conductance of azobenzene-containing molecules with trans and cis conformations was attributed to the difference in their lengths, different couplings to electrodes, and different tunneling pathways. The astonishing gate effect, as seen in Figure 2, on the transmission reveals new physics that requires explanation.

Electronic transport through molecules is usually governed by molecular orbitals, especially the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), those closest to the Fermi energy. Transmission by a molecular orbital exhibits a Lorentzian peak centered at approximately its energy and with width proportional to the strength of its coupling to electrodes. Both Gr | trans | Gr and Gr | cis | Gr junctions show two peaks in their transmission curves at zero gate voltage (Figure 3). Peaks at around −0.7 eV correspond to the HOMO and those near 1.0 eV are attributed to the LUMO. The peak corresponding to the HOMO in trans junctions is narrow and weak (the peak becomes more clear in a linear scale plotting), which indicates a weaker coupling between this orbital and graphene electrodes. The dips in the transmission curves near the Fermi energy are the results of the small density of states in graphene electrodes. We also examined the evolution of the transmission curves of Gr | trans | Gr and Gr | cis | Gr junctions under different gate voltages (Figure 4) as a function of energy. Note that the energy range in here is smaller than that in Figure 3 and transmission peaks due to LUMO and HOMO do not appear in this energy window.

The Dirac point of graphene electrodes shifts along with the gate voltage (arrows in Figure 4). Peaks in transmission close to the Fermi energy are responsible for the Gr | trans | Gr junction, showing a higher transmission than that of the Gr | cis | Gr junction at a positive gate voltage (Figure 2). Near the Fermi energy, these emergent peaks cannot be explained by molecular orbitals, which are far away from the Fermi energy.

Figure 2. Transmission at the Fermi energy as a function of gate voltage for Gr | trans | Gr and Gr | cis | Gr junctions.

Figure 3. Transmission as a function of energy for (top) Gr | trans | Gr and (bottom) Gr | cis | Gr junctions under zero gate voltage.

Figure 4. Transmission curves under different gate voltages of Gr | trans | Gr and Gr | cis | Gr junctions. The position of the Dirac point of the graphene lead is denoted by arrows.
Figure 5. Band structure of (a1)–(a3) Gr | trans | Gr and (b1)–(b3) Gr | cis | Gr junctions for gate voltages of (a1, b1) $\epsilon_{g}= -13.6 \times 10^{-3}$ C/m², (a2, b2) $\epsilon_{g}= 0$, and (a3, b3) $\epsilon_{g}= 13.6 \times 10^{-3}$ C/m². The bands contributed by the top graphene layer are highlighted in blue. The Fermi energy is denoted by the dashed line at 0 eV. The energy shift of the HOMO state and the Dirac point ($E_D$) of the top graphene layer by gate voltages is plotted in (c).

Do these peaks correspond to states emerging from molecule–graphene or molecule–molecule interactions at the interface? We looked into the electronic structure to identify the states responsible for the transmission peaks near the Fermi energy. With this question in mind, we built periodic structures of Gr | trans | Gr and Gr | cis | Gr whose unit cells are shown in the inset of Figure 1. Each unit cell contains one molecule and 3 × 3 primitive cells of top and bottom graphene, corresponding to the density of molecules observed in experiments. Band structures of Gr | trans | Gr and Gr | cis | Gr are shown in Figure 5a2,b2. The strongly dispersive bands spanning the whole energy range come from graphene layers. The bands contributed by the top graphene layer (bonded to the molecule via van der Waals interaction) are highlighted in blue to distinguish them from those of the bottom graphene layer. The Dirac point of both graphene layers is 0.15 eV above the Fermi energy, and both of them are hole-doped due to charge transfer with molecules. The molecular orbitals show up as nearly flat bands due to the large distances (≈7 Å) among molecules. The LUMO corresponds to the dispersionless band at 1 eV above the Fermi energy, whereas the HOMO falls at around −0.7 eV. The HOMO–LUMO energy gap is 1.74 eV for trans and 1.90 eV for cis molecules. The HOMO and LUMO in both trans and cis molecules are localized on the azobenzene ligand (Figure 6). For trans molecules, the HOMO is strongly localized between the two benzene rings, whereas the LUMO spreads over the whole azobenzene ligand (Figure 6a1,a3). The HOMO and LUMO of cis molecules have very similar spatial distributions (Figure 6b1,b3).

The state near the Fermi energy can be identified from the band structure. The weakly dispersive bands crossing the Fermi energy (Figure 5a2,b2) can be traced to the C–C bond between the molecule and the bottom graphene layer. The charge density corresponding to this state mainly resides on the bottom graphene layer and the phenyl ligand chemically bonded to it; thus, it is an interface state (Figure 6a2,b2). The energy of the interface state is very close to the Dirac point of the bottom graphene layer; this fact is independent of the size of the supercell. We did test calculations using bigger supercells containing one molecule and more than 3 × 3 graphene primitive cells. Results show that the interface state always appears near the Dirac point of the bottom graphene. This indicates that the energy of the interface state is determined by a local interaction between a molecule and the bottom graphene not caused by artifacts due to periodic boundary conditions. The x–y plane integrated charge densities corresponding to the HOMO, LUMO, and the interface state are plotted along the z direction in Figure 6c,d. The charge density of the interface state decays exponentially across the whole molecule because its energy is within the LUMO–HOMO gap of the molecule and the decay rate is faster than that of both LUMO and HOMO states. The surface state is well-coupled to the bottom graphene, whereas its coupling with the top graphene is quite weak. Electronic transport via the interface state can be well-described using the nonequilibrium Green’s function method mentioned above.

Gate voltages shift the bands of Gr | molecule | Gr junctions. Band structures at gate voltages of $\epsilon_{g}= -13.6, 0.0, and 13.6 \times 10^{-3}$ C/m² are shown in Figure 5a,b. The LUMO and HOMO states shift toward lower energy as the gate voltage changes from negative to positive, although the HOMO–LUMO energy gap remains unchanged. The energy shift of bands from the top graphene layer is visible by tracing the position of the Dirac point. These energy shifts are summarized in Figure 5c, where the LUMO state is not plotted because its energy is within the LUMO–HOMO gap of the molecule and the decay rate is faster than that of both LUMO and HOMO states. The surface state is well-coupled to the bottom graphene, whereas its coupling with the top graphene is quite weak. Electronic transport via the interface state can be well-described using the nonequilibrium Green’s function method mentioned above.
have a weaker influence on the orbitals of cis molecules. The band due to the C–C interface state is insensitive to the gate voltage because it contributes a large density of states around the Fermi energy. The bands from the bottom graphene layer are pinned by the C–C interface state, so they are also unchanged by gate voltages.

\[ \text{DISCUSSION} \]

We first discuss the connection between the electronic structure and transport properties. Energy shifts of molecular orbitals in response to gate voltages are reflected in the transmission curve. A negative gate voltage raises the HOMO closer to the Fermi energy (Figure 5). The enhancement of transmission of Gr cis | Gr junctions at negative energies is due to the tail of the Breit–Wigner resonance through the HOMO (Figure 4). (The Breit–Wigner resonance was first derived in the context of nuclear physics.\textsuperscript{48} A modern introduction of the Breit–Wigner resonance in electronic transport can be found in refs 49, 50.) This phenomenon is not observed in trans junctions because of the strongly localized HOMO. Positive gate voltages lower the LUMO closer to the Fermi energy, which results in a similar enhancement of transmission at positive energies. This enhancement happens only in the cis junction, in which gate voltages more efficiently tune the energies of molecular orbitals (Figure 5c).

Low-energy peaks in the transmission curve are closely related to the interface state. Positions of transmission peaks are not affected by gate voltages (Figure 4) because the energy of the interface state is insensitive to the gate voltage. The heights of transmission peaks are tunable by gate voltages. At zero gate voltage, the contribution of the interface state is canceled by the low density of states of the graphene leads, which results in the absence of transmission peaks (see the middle panel with \( \epsilon_0 = 0 \) of Figure 4). The gate voltage brings the interface state into play by shifting the Dirac point of the top graphene layer away from the Fermi energy, and transmission peaks emerge as a
result. However, the complexity of the resulting voltage dependence of the transmission curve goes far beyond a simple shift. The interface state contributes peaks in the transmission curve around the Fermi energy and dominates the transmission at positive gate voltages (Figure 4).

Next, we discuss the mechanism behind the dual peak in the transmission curve around the Fermi energy at a positive gate voltage (top panel, Figure 4). At first glance, the asymmetric dual peak is reminiscent of the Fano resonance, but it was excluded after detailed analysis. The Fano resonance mechanism involves two conducting channels separated in energy: a first (background) channel has an energy far away from the Fano region and a second (local) channel near the Fano region. Interference between the two channels results in an asymmetric transmission peak, and destructive interference can lead to a valley between two peaks. To apply Fano’s model to GrI molecule | GrI junctions, the interface state around the Fermi energy can be seen as the local channel. For the trans junction, the molecular LUMO can serve as the background channel, which contributes transmission at positive energies. This explanation however fails for the cis junction, which shows no signature of LUMO contribution to the transmission at positive energies. A novel interpretation is needed. We note that the interface state in Figures 6a2, b2 forms a band with a 0.2 eV width (Figures 5a, b) that is of the same order of magnitude as that of the width of the asymmetric peaks in the transmission. We hypothesize that the asymmetric transmission peak arises from interference of interface states. If true, the width and shape of the transmission peak can be changed by tuning the dispersion and width of the band corresponding to the interface state. We carried out supplementary calculations using the same configuration in Figure 1 but with the density of molecules reduced by half; the band dispersion of the interface state is thus also reduced. Calculations show that the width of the transmission peak is reduced and, more importantly, the dual-peak feature disappears (Figure 7). This supports our hypothesis that the asymmetric transmission peak is contributed by the interface state. This result can also be viewed as an evidence against the Fano mechanism because none of the global or local channels are killed by reducing the molecular density.

CONCLUSIONS

We studied a vertical field-effect system consisting of graphene and photoswitchable aryl azobenzene molecules. Light irradiation can transform the molecule between trans and cis conformations. Calculations demonstrate the simultaneous control of the electronic structure and transport properties by light irradiation and gate voltages. A gate voltage shifts the positions of the LUMO and HOMO of molecules and the bands from graphene. The C−C chemical bonding between molecules and the bottom graphene layer results in an interface state at the Fermi energy. This interface state interacts with other C−C bonding states can lead under a finite gate voltage to a strong peak at the Fermi level and therefore dominate the transport properties of junctions. The distinct feature of this junction, as shown in the calculated transmission curves (Figure 4), illustrates the importance of interfacial processes and predicts that emergent patterns in transmission functions can be engineered.

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Notes

The authors declare no competing financial interest.

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