Supplement Materials for

Simulating the Nanomechanical Response of Cyclooctateraene Molecules on a Graphene Device

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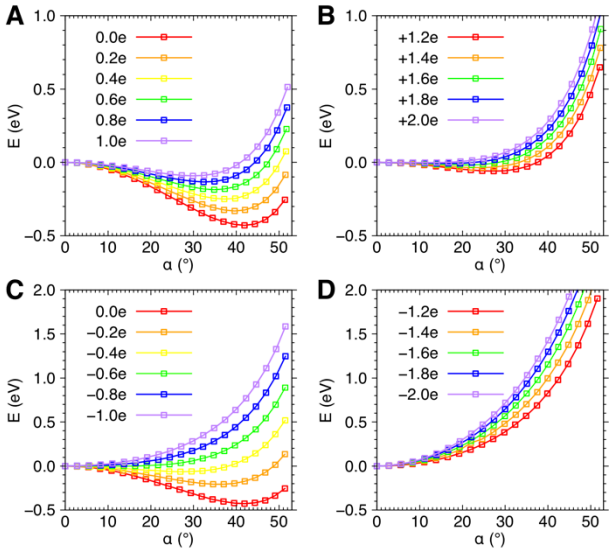

Fig. S1. Energy as functions of the bent angle and charge of a freestanding COT molecule. The total energies are plotted as functions of the bent angle (A,B) for positively and (C,D) negatively charged molecule.

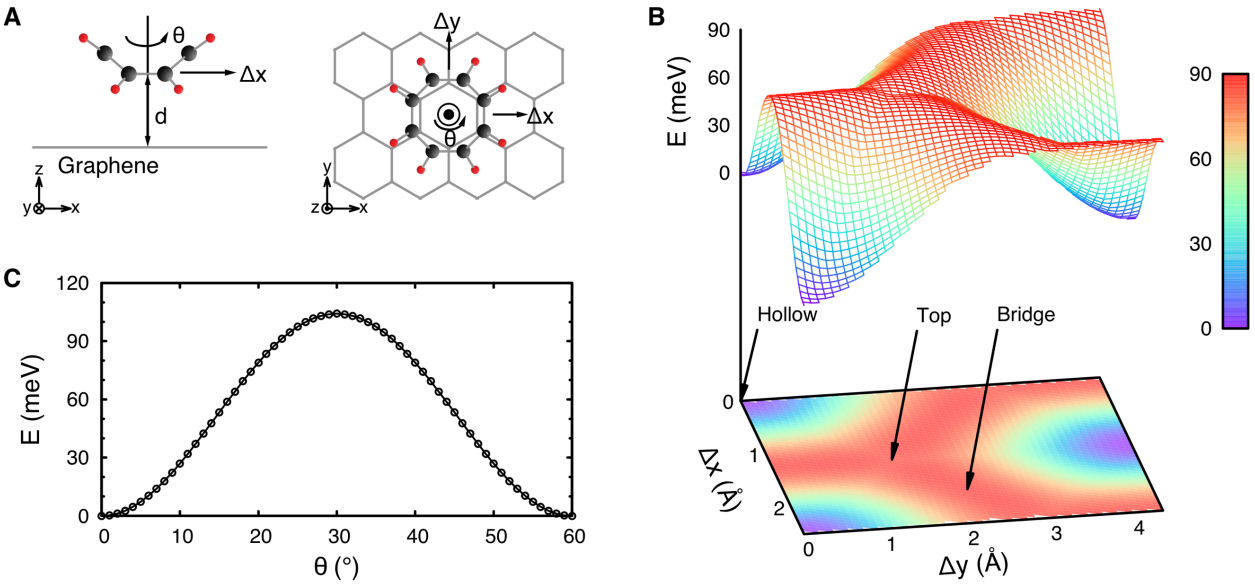

Fig. S2. Energy as functions of the parallel shift and rotation of a COT molecule adsorbed onto graphene. (A) The atomic structure of a COT molecule with a tub-shaped conformation adsorbed onto graphene is schematically illustrated. Side and top views are presented. The atomic structure is constructed using the atomic positions of the freestanding COT molecule and pristine graphene with a distance from the graphene surface to the bottom carbon atoms of the molecule d = 3.089 Å. The total energies are obtained as functions of (B) parallel shift, Δx and Δy, and (C) the rotational angle, θ, without further relaxing, where the origin, $\Delta x = \Delta y = \theta = 0$, is set to the position and orientation of the molecule shown in (A), and $E(\Delta x = \Delta y = \theta = 0)$ is set to zero.

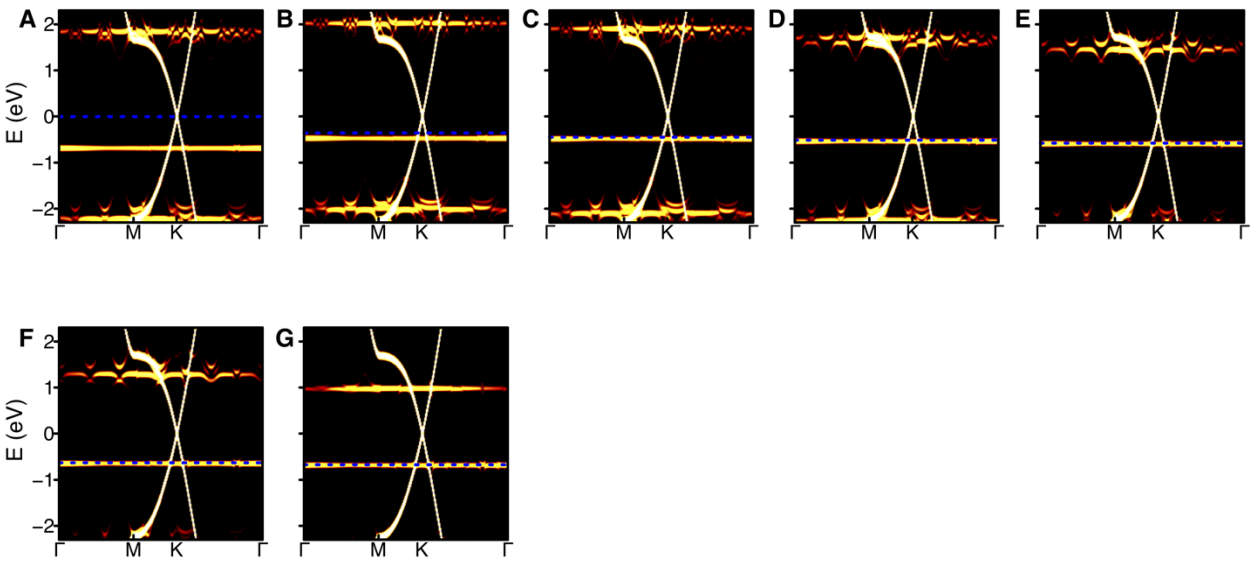

Fig. S3. The electronic band structures of a COT molecule on graphene with hole carrier density. The band structures with the carrier density of (A) 0, (B) $+1.47\times10^{13}$, (C) $+2.94\times10^{13}$, (D) $+4.41\times10^{13}$, (E) $+5.89\times10^{13}$, (F) $+7.35\times10^{13}$, and (G) $+8.82\times10^{13}$ e/cm^2 are shown, from left to right. The bands are unfolded with respect to the unit cell of graphene. The energies of Dirac points are set to zero and the Fermi energies are denoted by blue dashed lines.

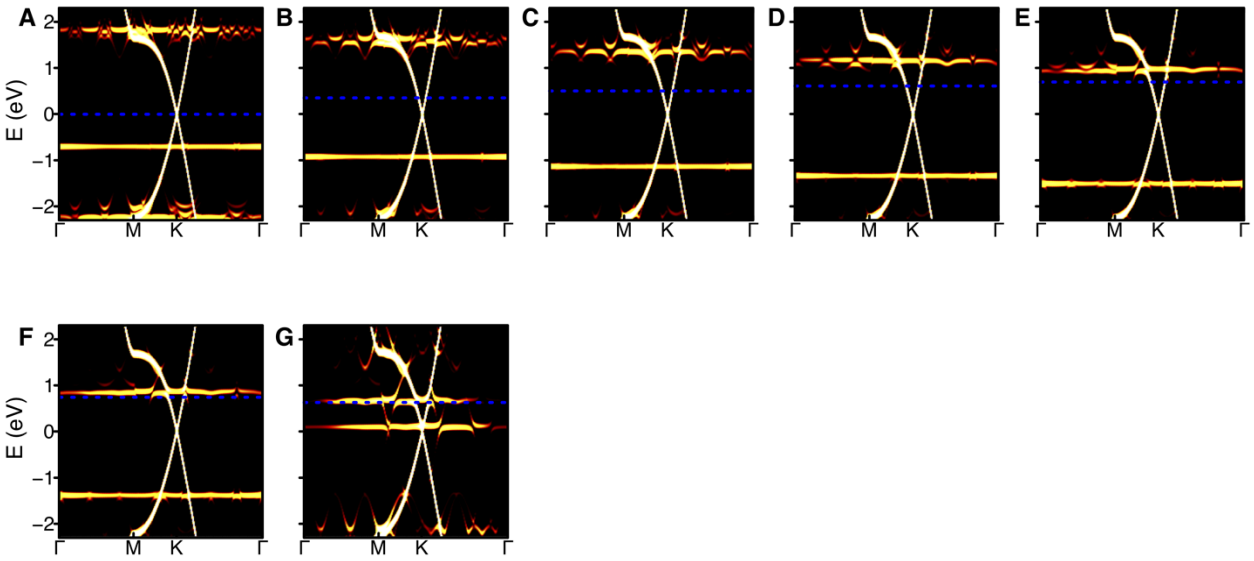

Fig. S4. The electronic band structures of a COT molecule on graphene with electron carrier density. The band structures with the carrier density of (A) 0, (B) -1.47×10^{13}, (C) -2.94×10^{13}, (D) -4.41×10^{13}, (E) -5.89×10^{13}, (F) -7.35×10^{13}, and (G) -8.82×10^{13} e/cm^2 are shown. The bands are unfolded with respect to the unit cell of graphene. The energies of Dirac points are set to zero and the Fermi energies are denoted by blue dashed lines.