Charge transport through dicarboxylic-acid-terminated alkanes bound to graphene-gold nanogap electrodes

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The dependence of transport properties on molecular length of the dicarboxylic-acid-terminated alkane in a graphene-molecule-gold junction (Gr-Au):

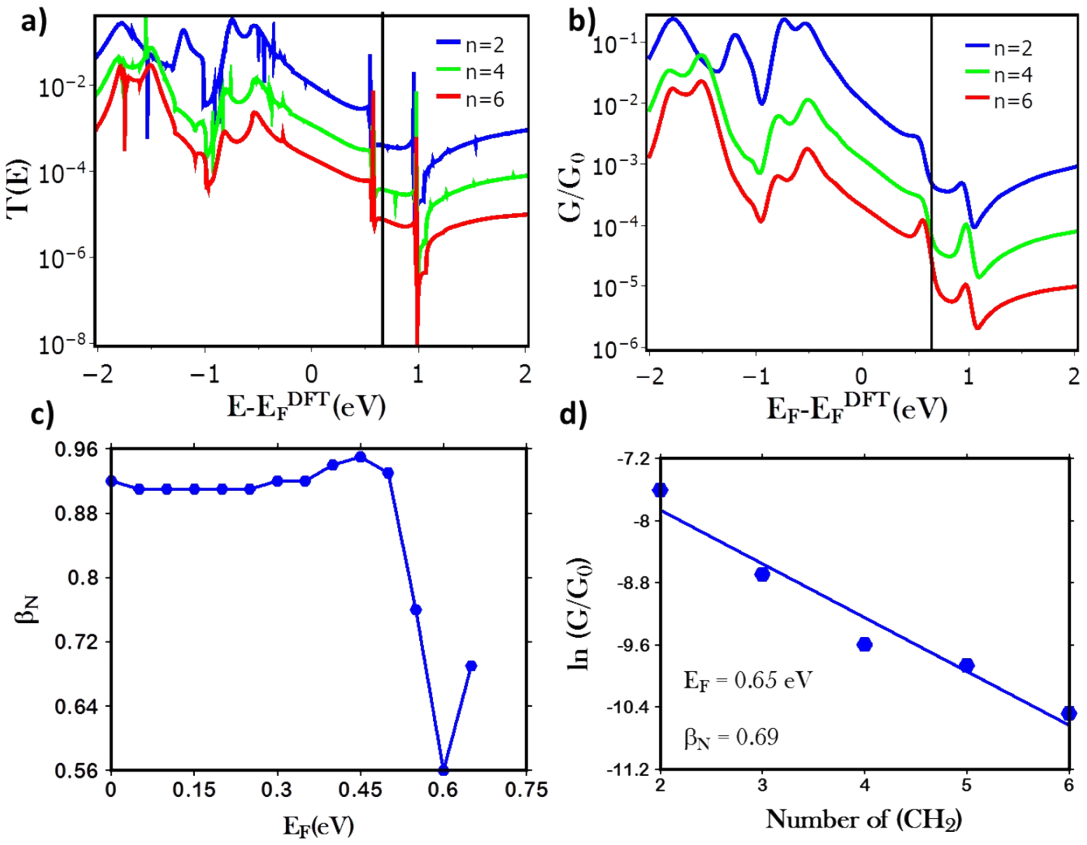

Figure S1. For the structures in Figure 5a-c, Figure S1 shows a) the transmission coefficients as a function of energy of the systems containing the dicarboxylic-acid-terminated alkane molecule with the

lengths n=2, n=4 and n=6 of CH_2 attached to the graphene-gold electrodes, b) demonstrates the room temperature electrical conductances over a range of Fermi energies, c) shows the room-temperature tunnelling factor β_N as a function of Fermi energy, and d) the logarithm of conductance versus the molecular length of the dicarboxylic-acid-terminated alkane.

Table S1. A comparison between the experimental measurements and DFT-CA calculations of the structures such as those shown in Figure 5.

Molecules	Conductance(G=I/V, nS)	
	Theoretical value, E_F= 0.65 eV	experimental value
$HOOC(CH_2)_2COOH$	38.5	15.6
$HOOC(CH_2)_4COOH$	5.3	5.0
$HOOC(CH_2)_6COOH$	2.2	1.08

Table S1 shows the theoretical and experimental conductances of three graphene-molecule-Au junctions. The conductances decrease with increasing molecular length.

Relaxed structures of dicarboxylic-acid-terminated alkanes placed between two gold electrodes (Au-Au):

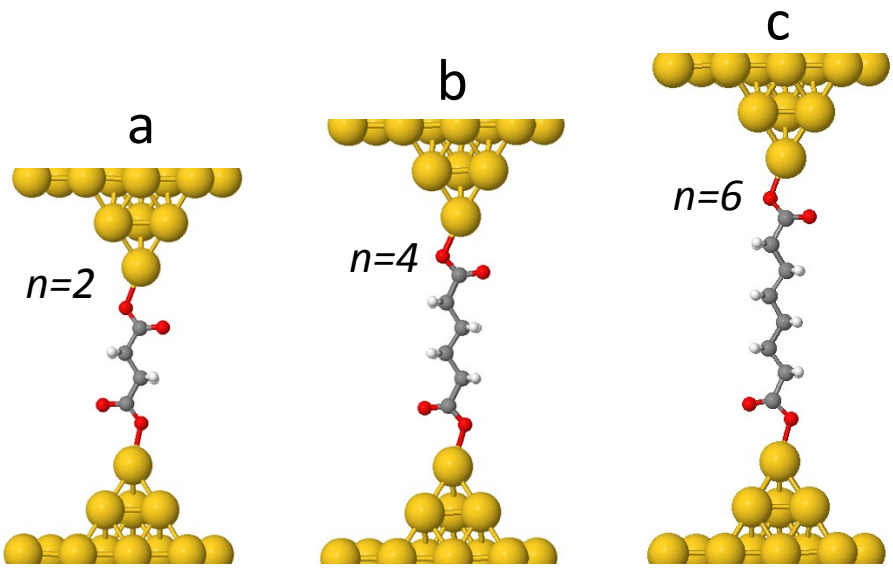

Figure S2. (a, b and c) show the optimized geometries of systems containing the dicarboxylic-acid-terminated alkanes of lengths (n=2, 4 and 6) connected to two gold electrodes.

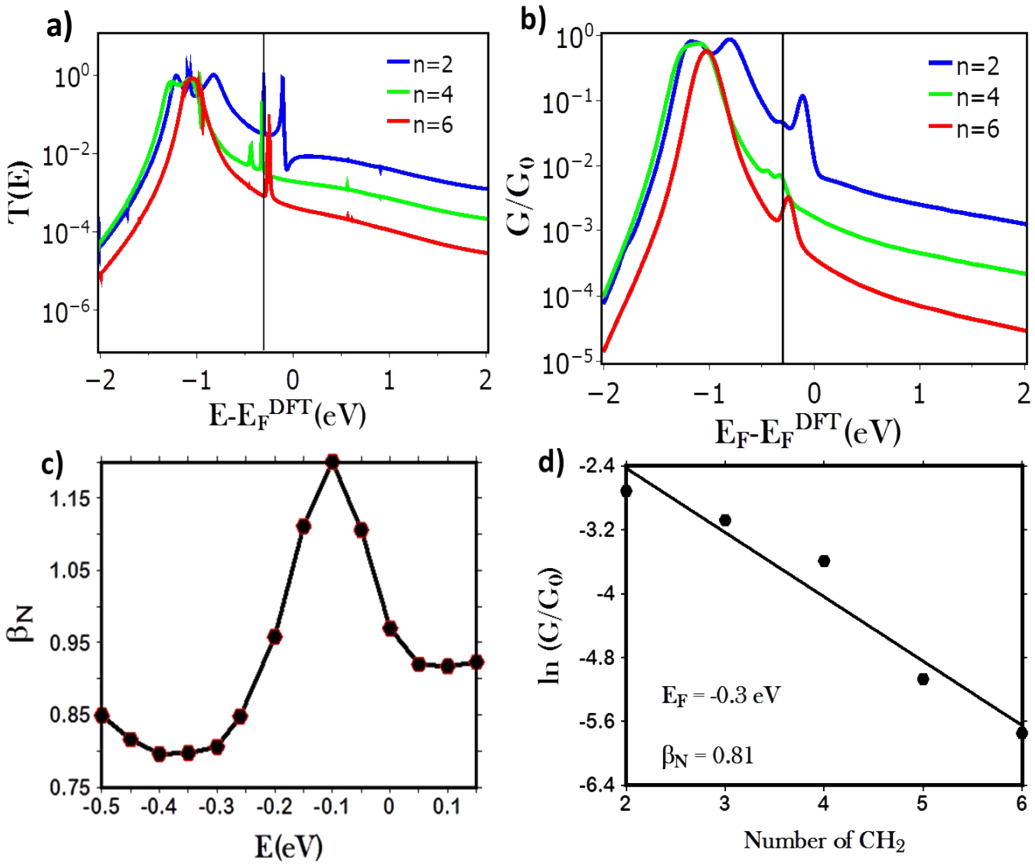

Figure S3. For the Au-molecule-Au structures in Figures S2a-c, Figure S3 shows a) the transmission coefficients as a function of energy b) the room temperature electrical conductances over a range of Fermi energies, c) the room-temperature attenuation factor β_N as a function of Fermi energy, and d) the logarithmic conductance versus the molecular length.

Theoretical results for defective graphene

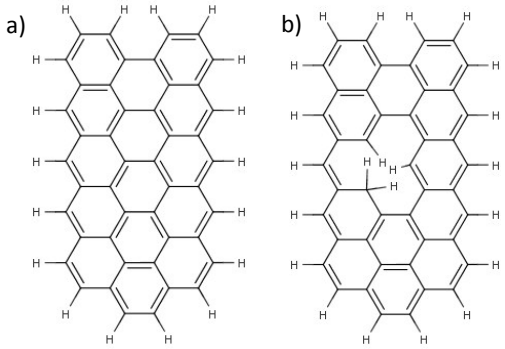

Figure S4. a) A perfect graphene sheet and b) a defected graphene sheet.

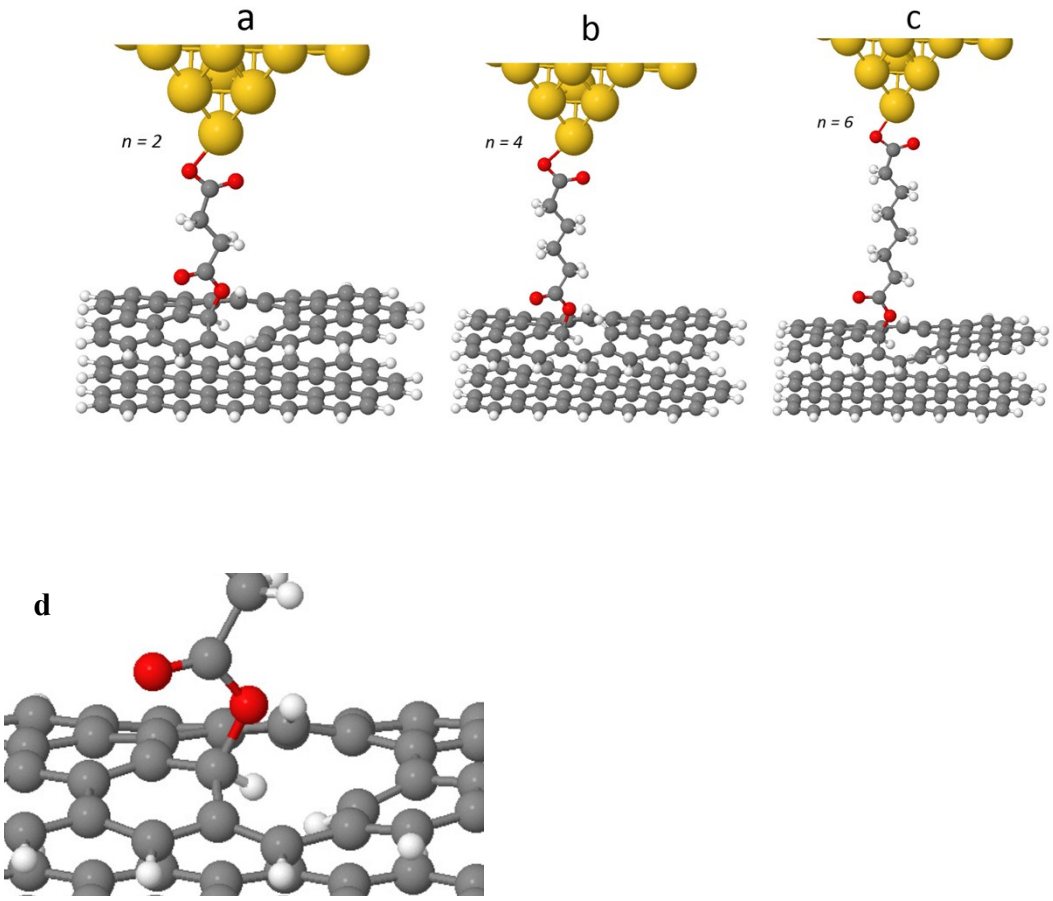

Figure S5. (a, b and c) show the optimized geometries of systems containing the dicarboxylic-acid-terminated alkanes of lengths (n=2, 4, and 6) connected to a defected graphene sheet. (d) Shows the detail of the defected graphene sheet.