

Supporting information for

Negative differential electrical resistance of a rotational organic nanomotor

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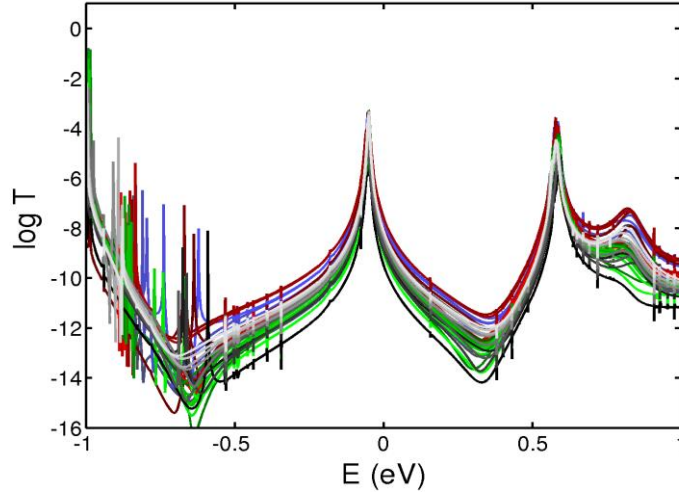
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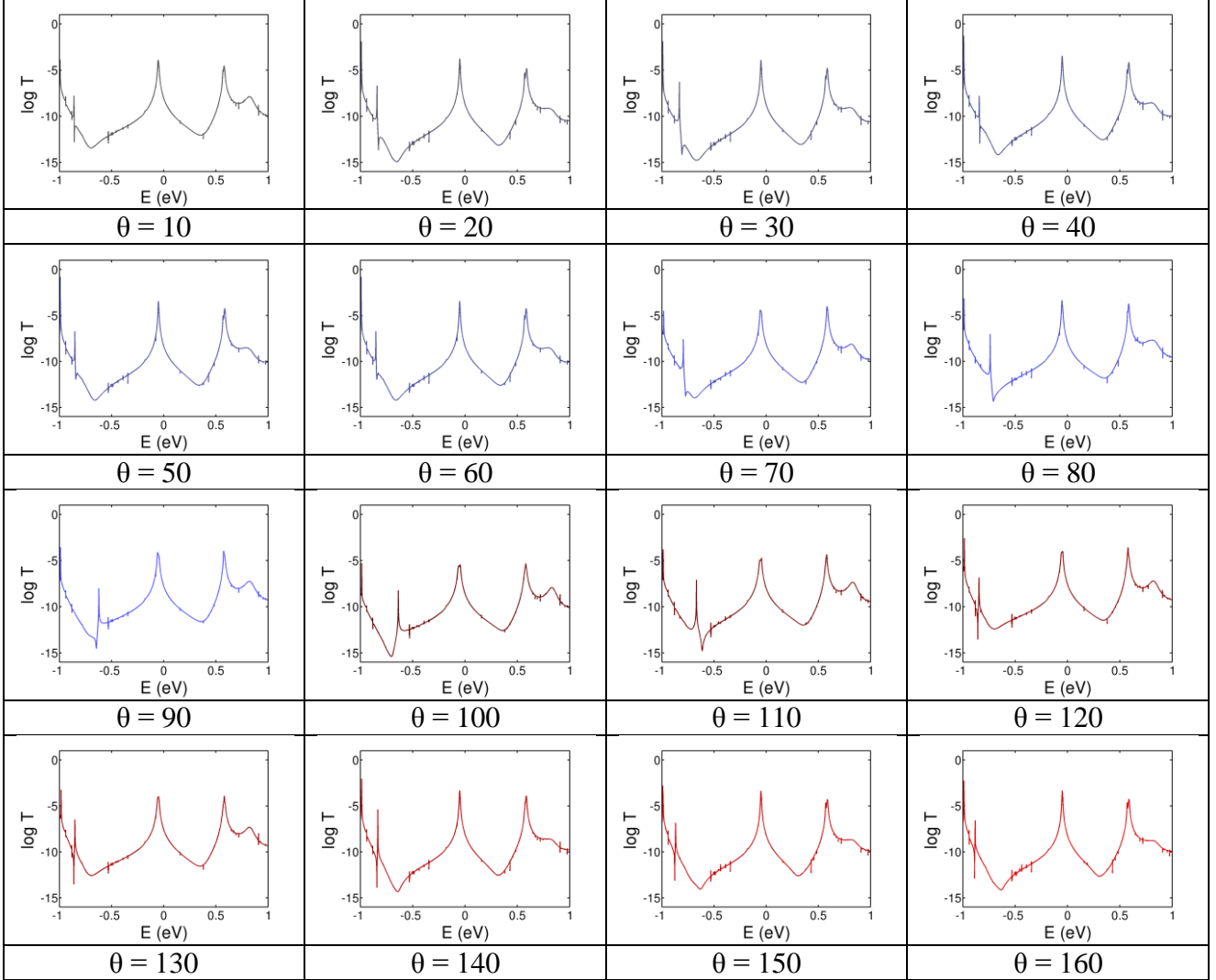
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Additional theoretical information



Transmission coefficient for full rotation of the rotor



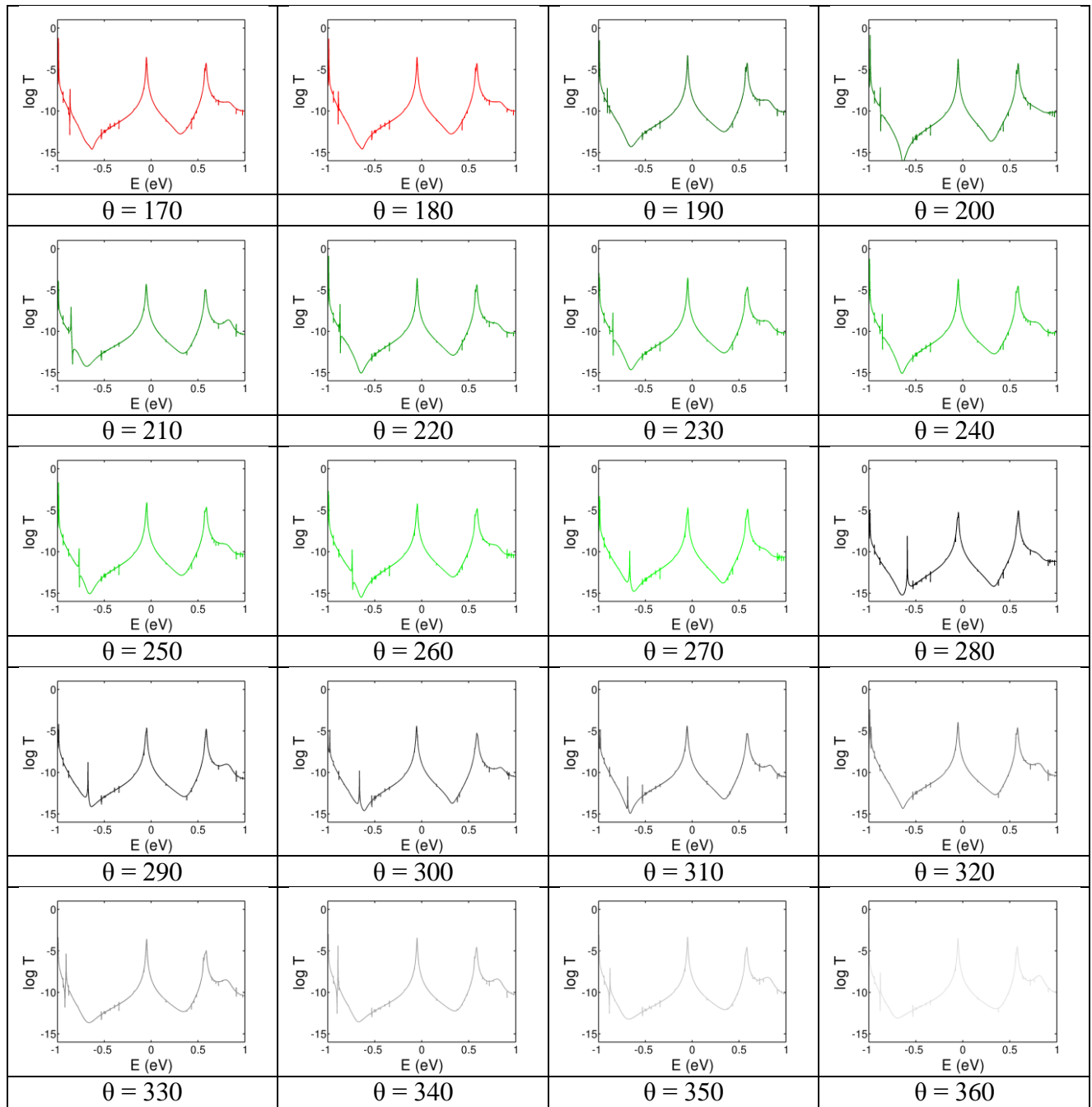


Figure S1: Transmission coefficient $T(E)$ of electrons with energy E passing from one fullerene to another for full rotation of the rotor.

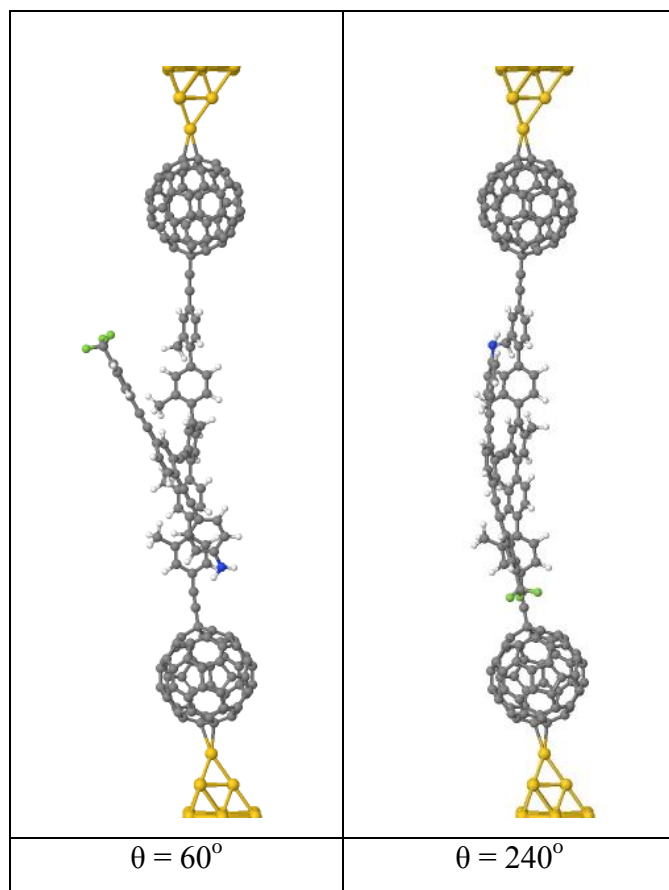


Figure S2: The molecular conformations corresponding to 60 and 240 degrees. Note that the pendant group is first rotated by θ and then the structure is relaxed. During geometry relaxation, the pendant group relax to the ground state which slightly changes the rotation angle θ .

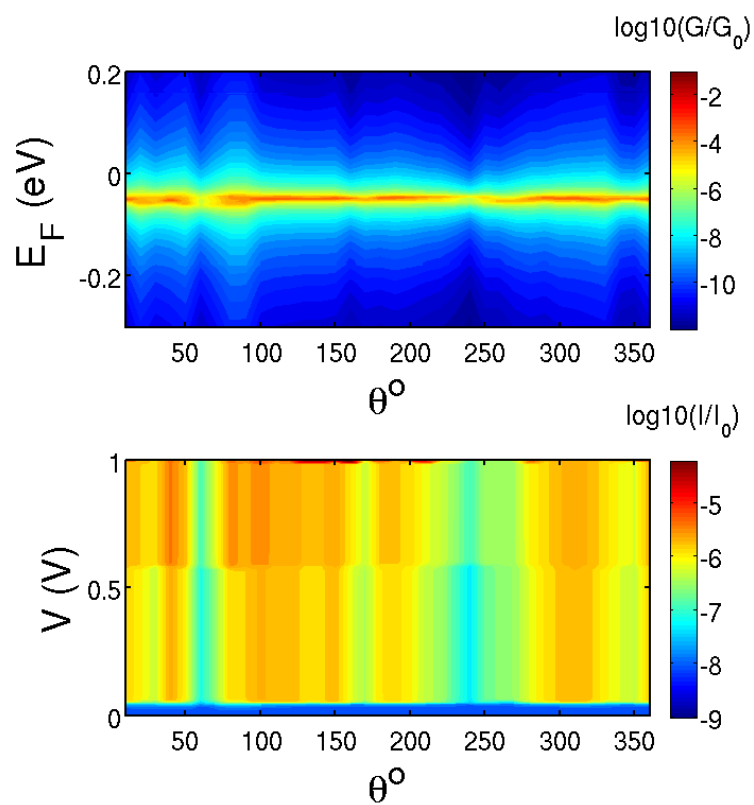


Figure S3: The contour plot of the conductance G/G_0 and current I/I_0 through the dumbbell molecule between two gold electrodes against angle θ and E_F (eV) at zero temperature.

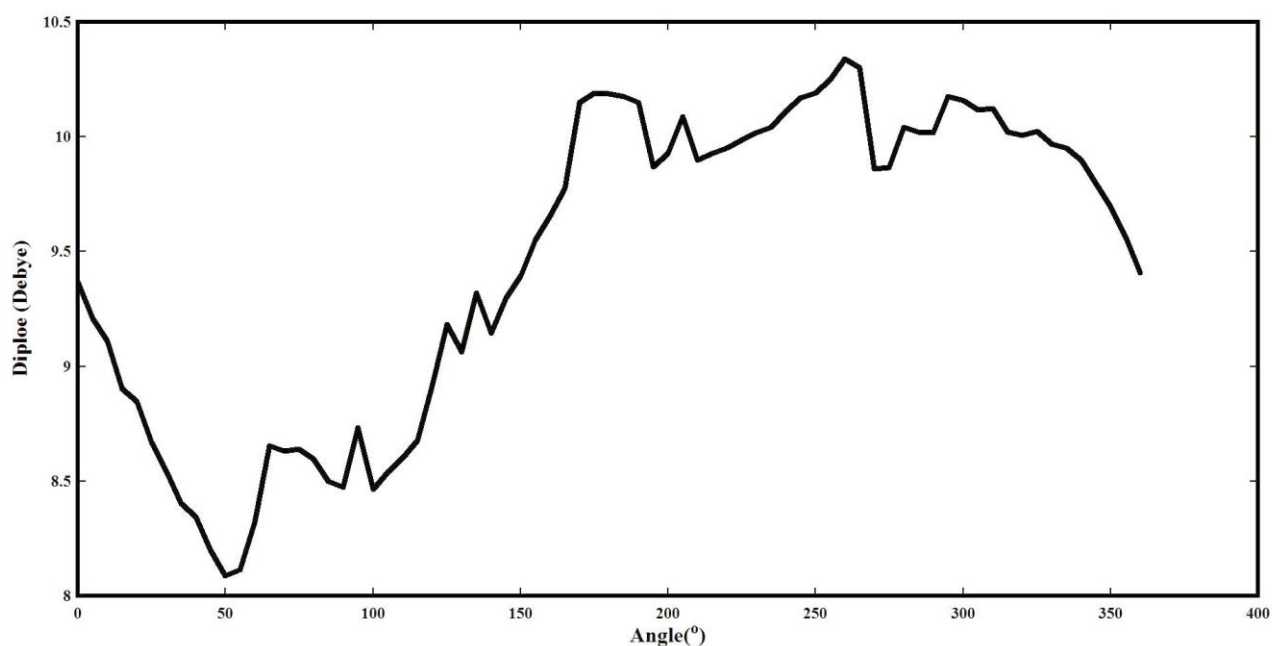


Figure S4: The dipole moment for the combined pendant group and backbone for all the rotation angles of the pendant group relative to the backbone is shown. The dipole moment shows oscillatory behaviour with a minimum at $\approx 50^\circ$ of ≈ 8.1 debye and a maximum at $\approx 240^\circ$ of ≈ 10.2 debye with an average of ≈ 9.4 debye. The length of the rotor and backbone is shown in Figure S5 to be 28.23 \AA .

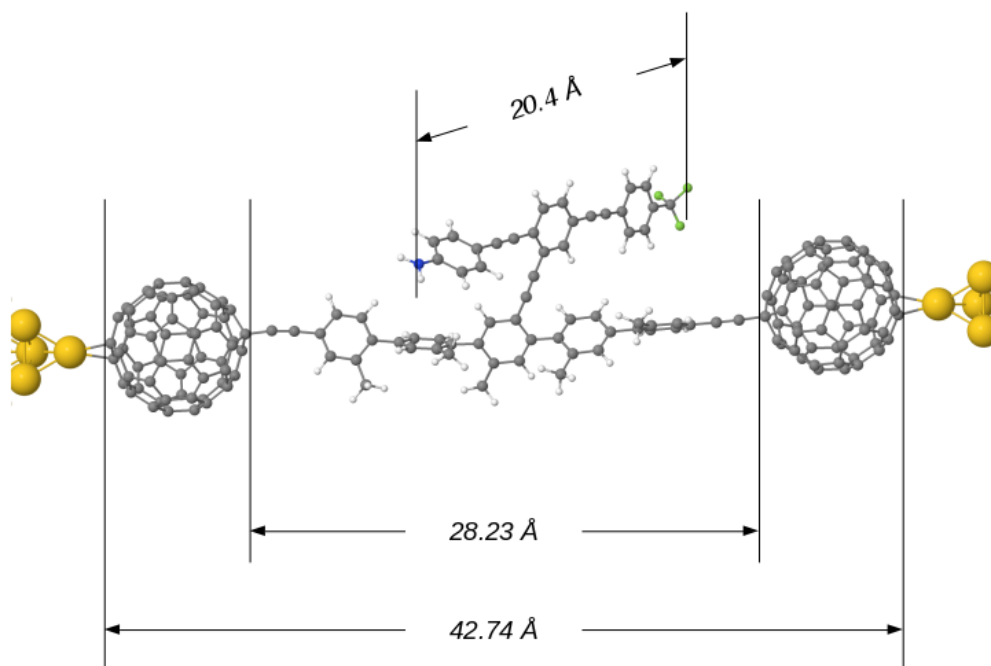


Figure S5: The length scales of the nanomotor.