

Supplementary Information for

Direct imaging of rotating molecules anchored on graphene

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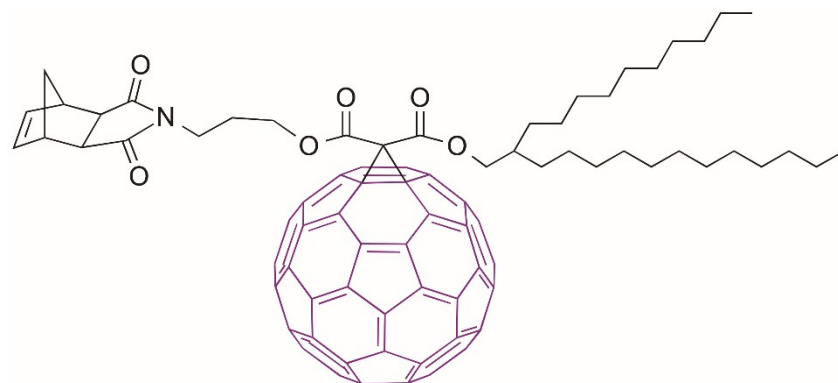
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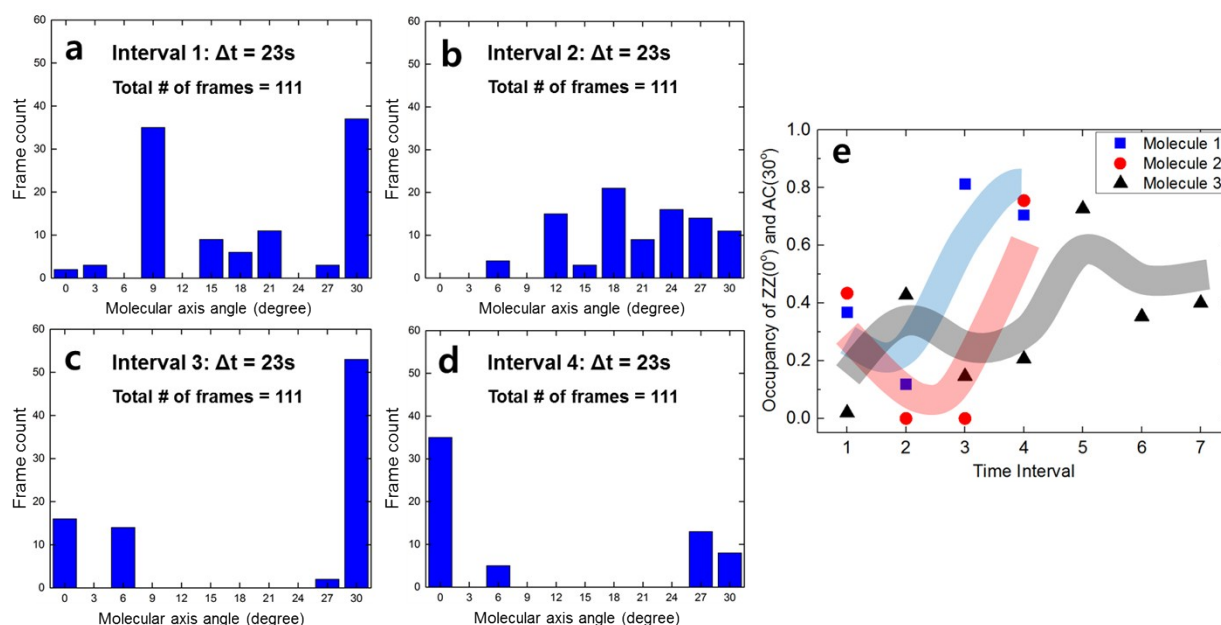
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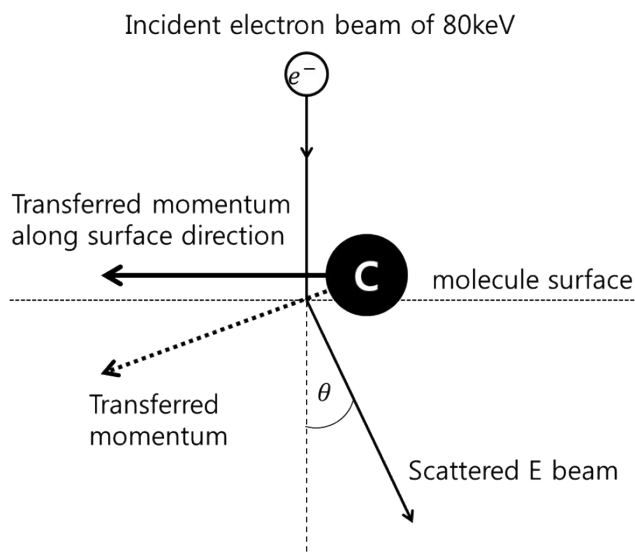
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Supplementary Figure S1. Structural formula of C_{60} -containing poly(norbornene) derivative ($m = 3$). The detailed synthesis of molecules can be found in the previous report.^{S1}



Supplementary Figure S2. Time-dependent molecular configurations. (a-d) Angular configuration of molecule 1 for sequential time intervals. (e) The time evolution of occupancy of zigzag(ZZ) and armchair(AC) configurations. The thick lines are guides to the eye.



Supplementary Figure S3. Elastic scattering geometry for surface-directional momentum transfer from incident electron beam to carbon atom in molecule.

Supplementary Table 1. The analyzed data set of molecules to estimate the rotational energy barriers.

Molecule #	Total # of atoms	Normalized event rate (s ⁻¹)	Surface energy barrier threshold (eV)	Energy barrier (meV / atoms)	Energy barrier per C ₆₀ (meV / C ₆₀ molecule)
1	114	1.7±0.8	0.27	2.4 1.6 (lower limit) 4.7 (upper limit)	1.4×10^2 9.7×10^1 (lower limit) 2.8×10^2 (upper limit)
2	267	2.7±0.8	0.40	1.5 1.1 (lower limit) 2.1 (upper limit)	8.9×10^1 6.8×10^1 (lower limit) 1.3×10^2 (upper limit)
3	279	0.15±0.10	3.3	12 9.6 (lower limit) 14 (upper limit)	7.0×10^2 5.8×10^2 (lower limit) 8.2×10^2 (upper limit)

Supplementary Note 1

The Coulomb scattering theory for calculating event rate

The differential cross section of elastic scattering^{S2} when surface transferred energy E is given can be written as

$$\frac{d\sigma(E)}{dE} = \frac{\pi Z^2 \gamma^2}{k_0^4 a_0^2 E_{max} \left(1 - \sqrt{1 - \frac{E}{E_{max}}}\right)^2 \sqrt{1 - \frac{E}{E_{max}}}} \quad (S1)$$

where Z is the atomic number of the target atoms, $\gamma = (1 - v^2/c^2)^{-1/2}$ the Lorentz factor, k_0 the incident-electron wavenumber, a_0 and the Bohr radius of the hydrogen atom ($5.3 \times 10^{-11} m$). E_{max} is the maximum surface transferred energy and can be written as

$$E_{max} = \frac{E_0(E_0 + 2m_e c^2)}{2Mc^2} \quad (S2)$$

under the assumption that the target atom mass M is much heavier than the electron mass m_e (E_0 is the kinetic energy of the incident electron). At 80 kV TEM operation, E_{max} is 3.95 eV for carbon atoms.

Supplementary References

S1. Fang, L.; Liu, P.; Sveinbjornsson, B. R.; Atahan-Evrenk, S.; Vandewal, K.; Osuna, S.; Jimenez-Oses, G.; Shrestha, S.; Giri, G.; Wei, P.; Salleo, A.; Aspuru-Guzik, A.; Grubbs, R. H.; Houk, K. N.; Bao, Z., Confined organization of fullerene units along high polymer chains. *J. Mater. Chem. C* **2013**, *1* (36), 5747-5755.

S2. Egerton, R. F., Beam-induced motion of adatoms in the transmission electron microscope. *Microsc. Microanal.* **2013**, *19* (2), 479-86.