— Supporting Information —

The Smallest Archimedean Screw: Facet Dynamics and Friction in Multi-Walled Nanotubes

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PES OF CARBON-BASED SYSTEMS

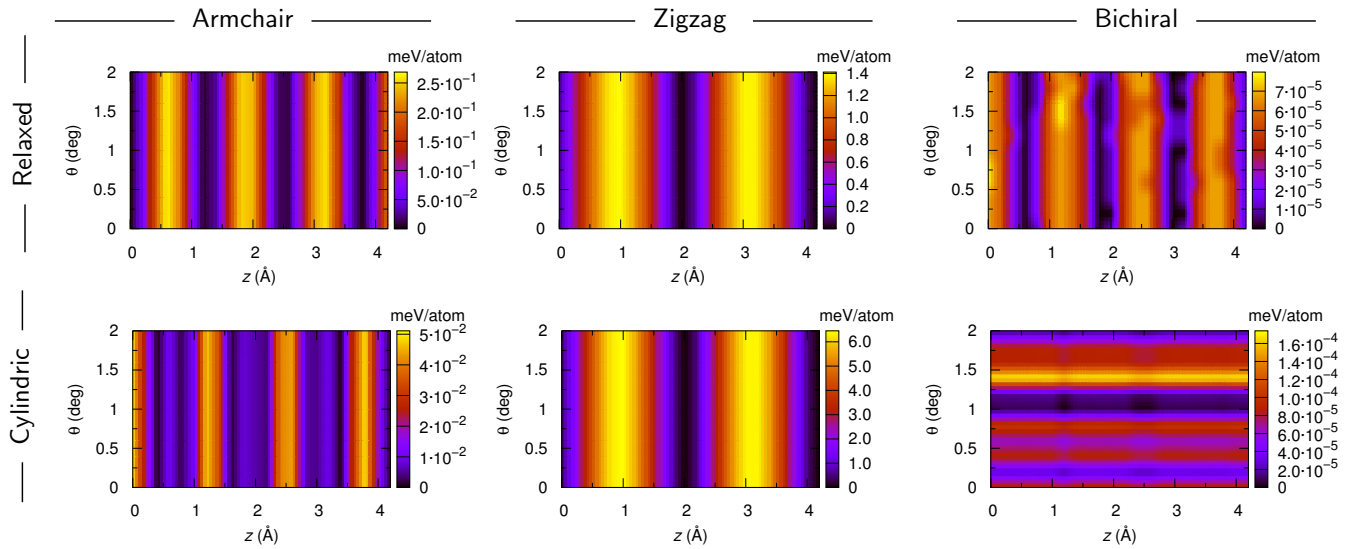

FIGURE S1: PES maps (Carbon) – Potential energy surface maps of the considered armchair (left column), zigzag (center column), and bi-chiral (right column) DWCNTs for relaxed (top panels) and cylindric (bottom panels) configuration.

FITTING STATIC FRICTION

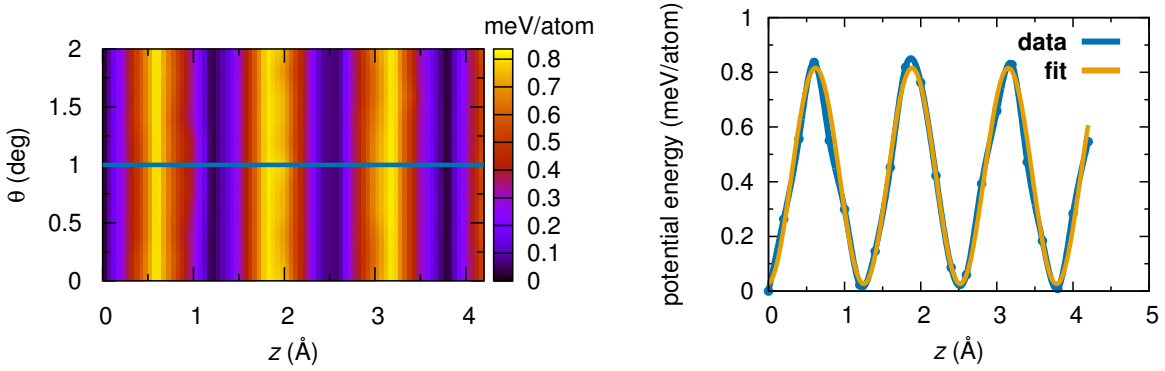

FIGURE S2: PES map for the armchair DWBNNT (left) and its corresponding E_z profile at $\theta = 1.0^\circ$ (right) alongside a sinusoidal fit. In an idealized case, obtained by assuming an equal force applied to all outer tube atoms and a compensating force to all inner tube atoms, the static friction force F_s can be estimated from the corrugation energy profile (i.e. the $E(z)$ at a fixed θ) by dividing the maximum energy excursion by the corrugation periodicity, $F_s = \pi E_c/\Delta z$, an approach which is exact in the case of a sinusoidal corrugation profile: $E(z) = (E_c/2)\sin(2\pi z/\Delta z)$.

EFFECT OF PARTIAL CHARGES ON CORRUGATION

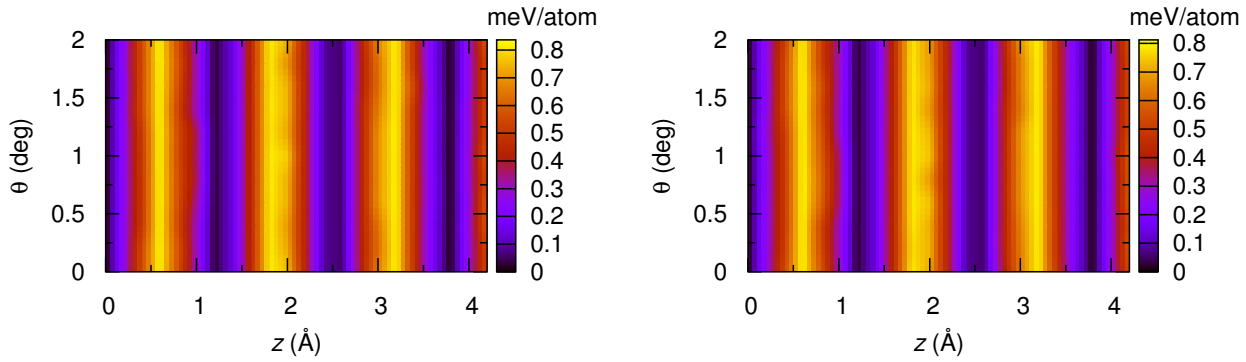

FIGURE S3: PES map for the (104,104)@(109,109) armchair DWBNNT, relaxed in the presence (left) of the partial charges on the B ($q_B = +0.47\,e$) and N ($q_N = -0.47\,e$) atoms, or in their absence (right, $qB = qN = 0$). The corrugation energy (E_{max} - E_{min}) of 0.84 meV/atom obtained in the charged system reduces to 0.81 meV/atom in the uncharged one.

CORRUGATION AND ADHESION ENERGY PROFILES

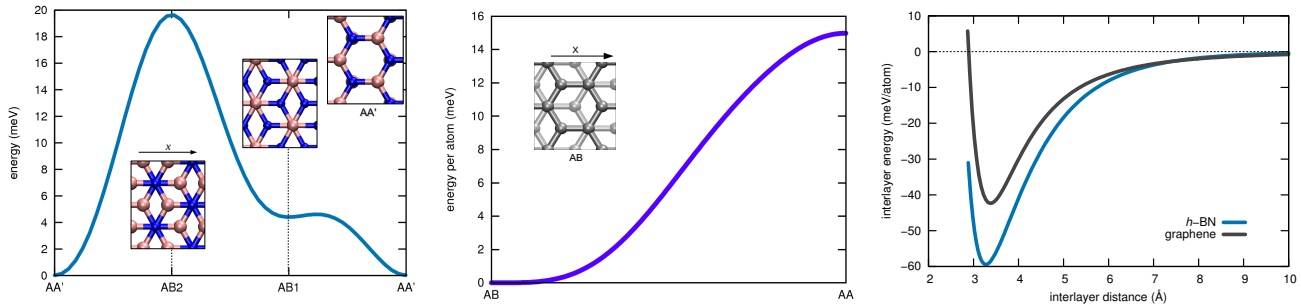

FIGURE S4: Potential energy profile for bilayer *h*-BN (left panel) or bilayer graphene (middle panel), calculated by rigidly shifting the top layer along the armchair direction x. The corresponding binding energy curves, obtained by rigidly shifting the top layer along the vertical direction at the AA' and AB stacking modes for *h*-BN and graphene, respectively, appear in the right panel. The resulting inter-layer binding energy for a graphene bilayer, 42 meV/atom, determined by the Kolmogorov-Krespi RDP1 potential, is comparable with the values reported in literature, ranging from 31 to 52 meV/atom.[1–5] For the *h*-BN bilayer our calculted adhesion energy of 59.4 meV/atom is compatible with *ab initio* DFT+vdW and Quantum Monte Carlo calculations reporting a range of 40.5–76.2 meV/atom.[6–8] Furthermore, our calculated corrugation values and trends are in line with reference values.[8,9] For the sake of clearness we note that the reported per-atom adhesion and corrugation values have been obtained by dividing the total energy by the number of atoms in one layer.

VELOCITY DEPENDENCE OF FRICTION

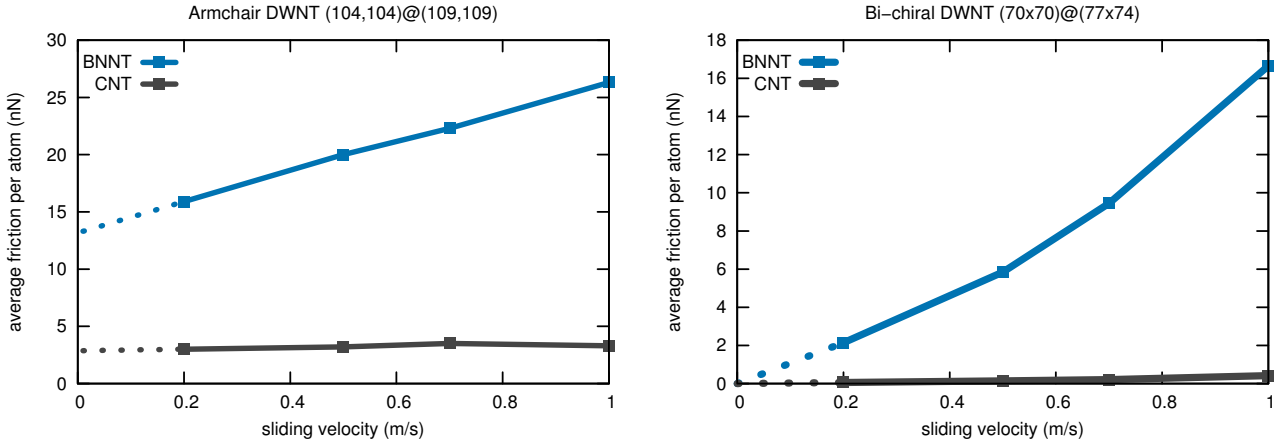

FIGURE S5: Average friction force obtained during telescopic sliding for the (104,104)@(109,109) armchair DWNTs (Left) and the (70,70)@(77x74) bi-chiral DWNTs (right) at different sliding velocities. In agreement with the experimental findings[10] DWBNNTs present consistently higher friction forces than DWCNTs of the same type with a viscous-like dependence on the sliding velocity. Note that in the armchair case the commensuration along the NT axis leads to a finite friction in the zero-velocity limit (dashed line), which is related to the static friction force – the latter clearly present for commensurate interfaces. Conversely, the incommensurate bi-chiral systems present a vanishing friction in the limit $v \to 0$, typical of a superlubric interface.

STATIC FRICTION AND CORRUGATION ENERGY

TABLE S1 – maximum inter-wall static friction force F_s (in meV/Å per atom), maximum corrugation energy (in meV per atom) for the cylindric (E_c^{cyl}) and relaxed (E_c^{relax}) configurations, and their difference ΔE_c, as calculated for the DWNTs considered.

	BN				C			
	F_s	E_c^{cyl}	E_c^{relax}	ΔE_c	F_s	E_c^{cyl}	E_c^{relax}	ΔE_c
AC@AC	1.91	$7.41{\cdot}10^{-2}$	0.84	0.77	0.66	0.05	0.27	0.22
ZZ@ZZ	2.04	8.41	1.45	-6.96	2.00	6.45	1.41	-5.04
AC@Ch	$3.87{\cdot}10^{-3}$	$0.13{\cdot}10^{-3}$	$2.29{\cdot}10^{-3}$	$2.16{\cdot}10^{-3}$	$0.18{\cdot}10^{-3}$	$17.4{\cdot}10^{-5}$	$7.96{\cdot}10^{-5}$	$-9.44{\cdot}10^{-5}$
ZZ@AC	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

STRUCTURAL PROPERTIES FOR THE SET OF CONSIDERED DWNTs

TABLE S2 – Chiral angle difference ($\Delta\Theta$), average diameter (D), interlayer spacing (d), and displacement from optimal interlayer spacing (d - d_{opt}) of the unrelaxed cylindrical DWNTs considered.

			BN			C		
System	Chiral indices	$\Delta\Theta$ (deg)	D (nm)	d (nm)	d - d_{opt} (nm)	D (nm)	d (nm)	d - d_{opt} (nm)
AC@AC	(104,104)@(109,109)	0.0	15.0	0.344	0.017	15.0	0.344	0.007
ZZ@ZZ	(180,0)@(188,0)	0.0	14.9	0.318	-0.009	14.9	0.318	-0.019
AC@Ch	(70,70)@(77x74)	0.657	10.4	0.378	0.051	10.4	0.378	0.041
ZZ@AC	(179,0)@(108,108)	30.0	14.9	0.321	-0.006	14.9	0.321	-0.016

MOVIE CAPTIONS

MOVIE 1: Cross sectional view of armchair (top panels) and Zigzag (bottom panels) DWNTs for BN (left panels) and carbon (right panels), relaxed at different relative axial positions z. Atoms are colored as a function of the inter-layer potential energy.

MOVIE 2: Cross sectional view of the armchair DWBNNT relaxed at different relative axial positions z (left) and dynamically driven at relative pulling velocity $v_z = 0.01$ Å/ps (right). Atoms are colored as a function of the inter-layer potential energy.

MOVIE 3: Dynamical view of the bi-chiral DWBNNT at relative pulling velocity $v_z = 0.01$ Å/ps. Atoms are colored as a function of the inter-layer potential energy.

MOVIE 4: Dynamical view of the bi-chiral DWCNT at relative pulling velocity $v_z = 0.01$ Å/ps. Atoms are colored as a function of the inter-layer potential energy.

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