Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supplementary Information

Robust nanotube-based nanosensor designed for the detection of explosive molecules

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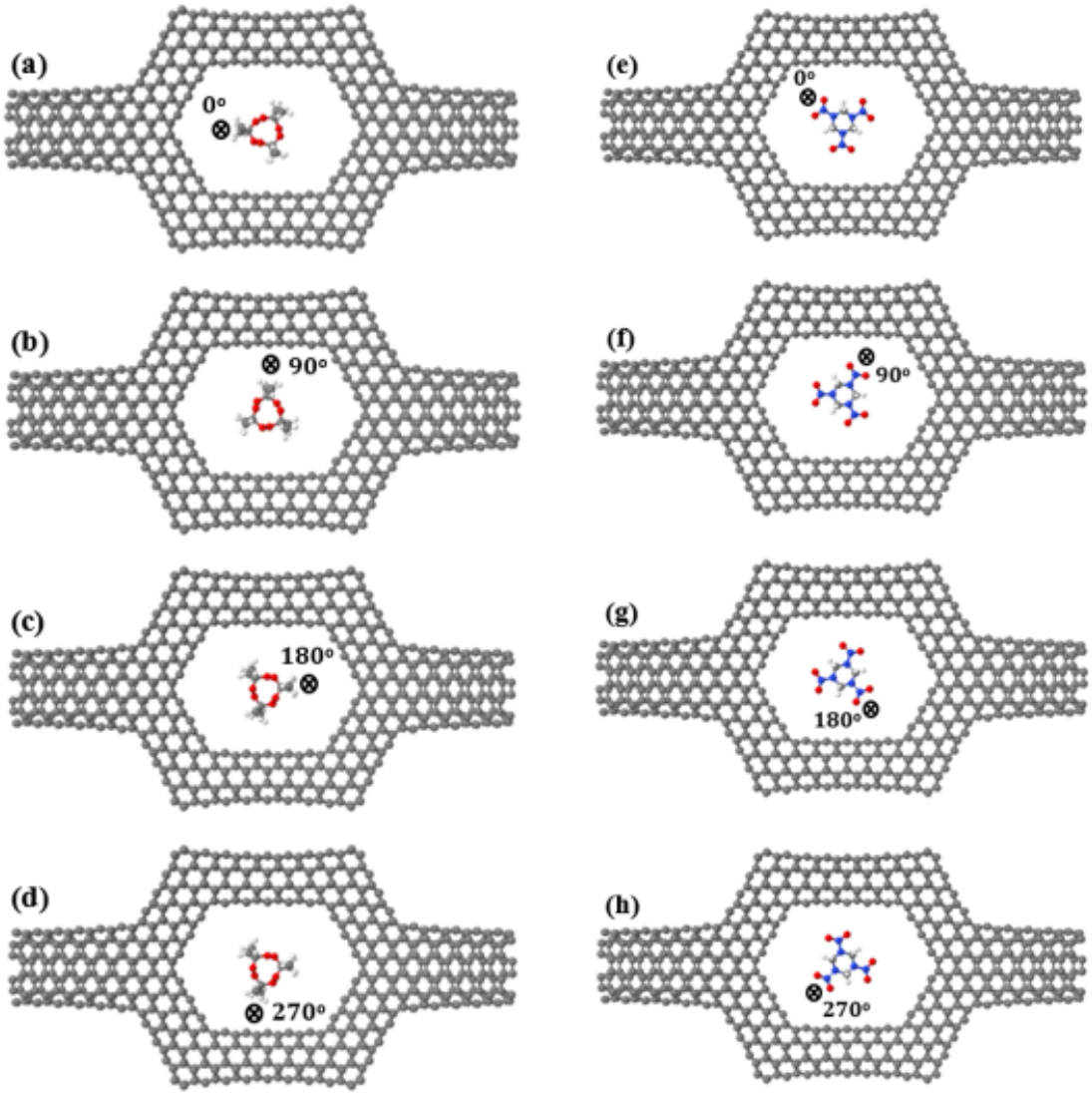

Figure S1: (a-d) Relaxed *Tor*+TATP with 0°, 90°, 180°, and 270°, respectively, and **(e-h)** Relaxed *Tor*+RDX with 0°, 90°, 180°, and 270°, respectively. In all subfigures, the circle with the diagonal cross symbol denotes the angle of orientation.

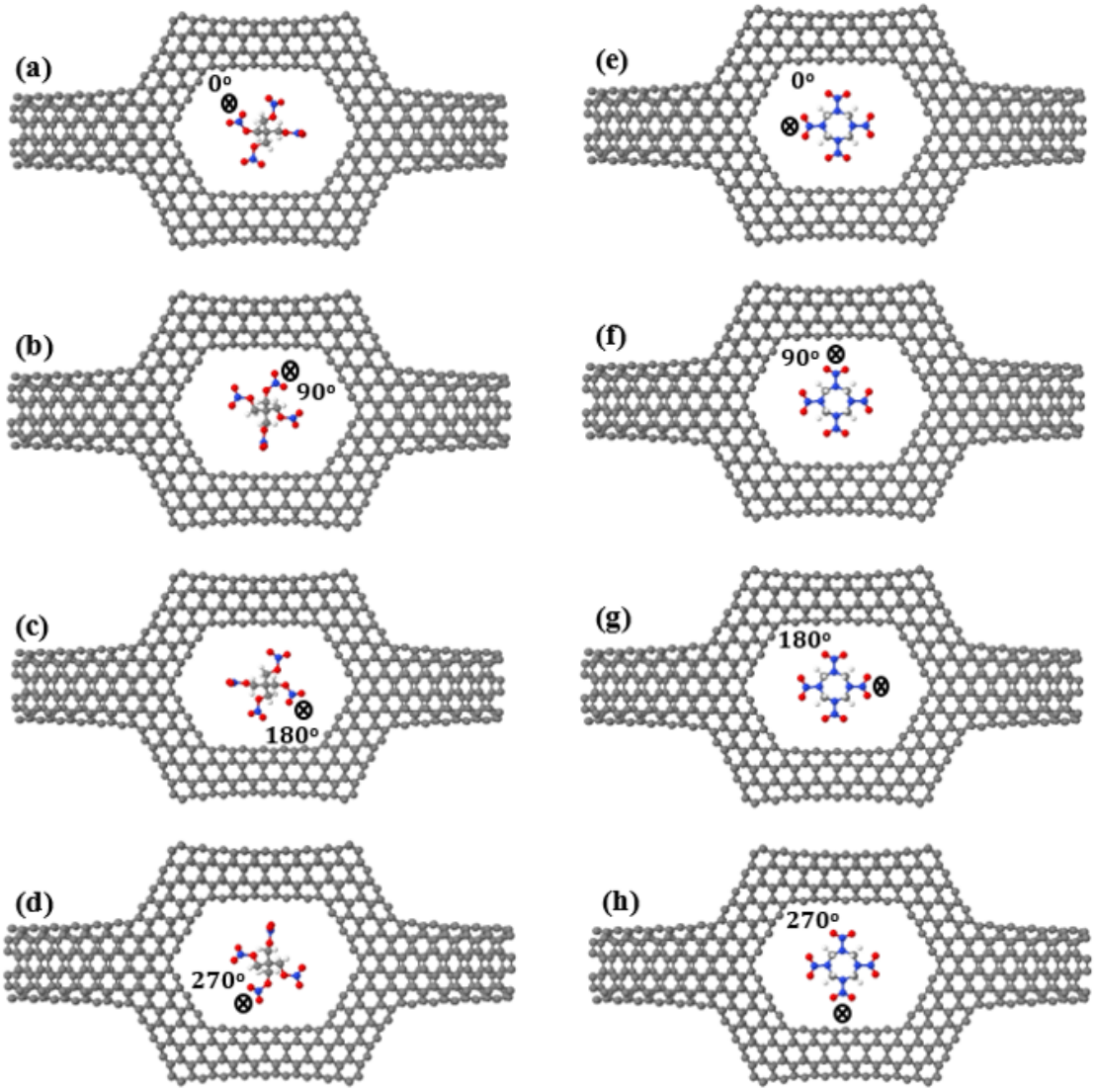

Figure S2: (a-d) Relaxed *Tor*+PENT with 0°, 90°, 180°, and 270°, respectively, and **(e-h)** Relaxed *Tor*+HMX with 0°, 90°, 180°, and 270°, respectively. In all subfigures, the circle with the diagonal cross symbol denotes the angle of orientation.

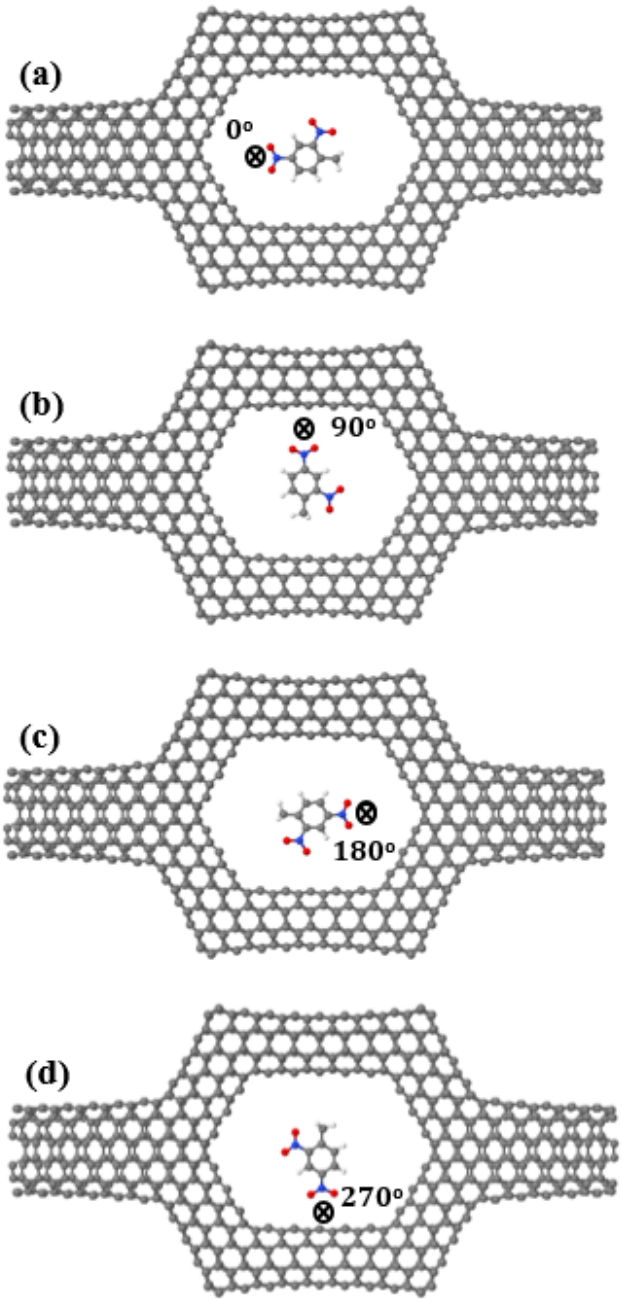

Figure S3: (a-d) Relaxed *Tor*+DNT with 0°, 90°, 180°, and 270°, respectively. In all subfigures, the circle with the diagonal cross symbol denotes the angle of orientation.

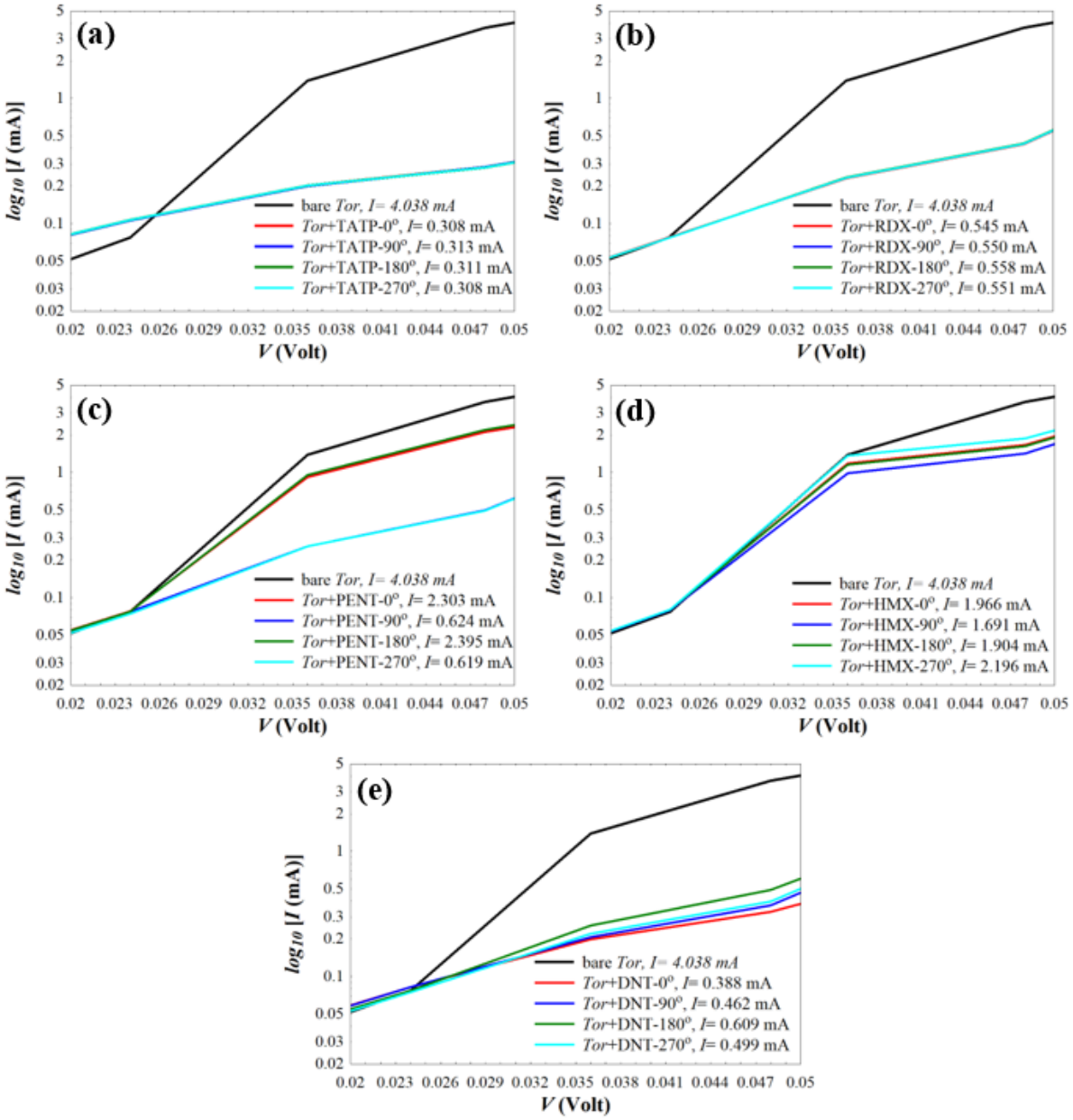

Figure S4: (a-e) Current (*I*) of the bare *Tor*, *Tor* +TATP, *Tor* +RDX, *Tor* +PENT, *Tor* +HMX, and *Tor*+DNT respectively. Each explosive molecule rotates with four angles of orientation inside the hollow region of the *Tor* (0°, 90°, 180°, and 270°).

Table S1: Distance between the inner walls of the nanopore and the closest atoms (H and O) of the explosive molecules at each orientation angle.

	Distance in angstrom (Å)			
Tor	Upper edge	Lower edge	Right edge	Left edge
+TATP-0°	H= 4.84	H= 4.41	H= 7.57	H= 7.15
+TATP-90°	H= 4.97	H= 4.52	H= 7.36	H= 6.99
+TATP-180°	H= 4.80	H= 4.12	H= 7.38	H= 7.29
+TATP-270°	H= 4.68	H= 4.13	H= 7.84	H= 7.27
+RDX-0°	H= 4.99 O= 4.64	H= 6.87 O= 4,86	H=8 .73 O= 7.35	H=7.87 O= 7.57
+RDX-90°	H= 5.32 O= 3.95	H= 6.13 O= 4.70	H= 8.36 O= 7.14	H= 8.76 O= 6.70
+RDX-180°	H=5.73 O= 3.96	H=6.13 O= 5.20	H=8.36 O= 7.55	H=8.27 O= 6.93
+RDX-270°	H= 6.27 O= 4.05	H= 5.69 O= 4.97	H= 9.00 O= 7.26	H= 7.67 O= 6.76
+PENT-0°	H= 5.72 O= 4.15	H= 5.64 O= 3.97	H= 8.44 O= 5.99	H= 9.70 O= 6.30
+PENT-90°	H= 6.84 O= 3.70	H= 6.79 O= 3.51	H= 8.13 O= 6.53	H= 8.50 O= 6.57
+PENT-180°	H= 5.51 O= 3.92	H= 6.13 O= 4.24	H= 9.16 O= 5.74	H= 9.01 O= 6.54
+PENT-270°	H= 6.10 O= 4.44	H= 7.00 O= 3.43	H= 7.94 O= 6.03	H= 8.70 O= 7.03
+HMX-0°	H= 5.67 O= 4.13	H= 5.57 O= 3.97	H= 8.56 O= 6.84	H= 8.03 O= 6.23
+HMX-90°	H= 5.72 O= 3.93	H= 5.55 O= 3.97	H= 8.57 O= 6.90	H= 8.00 O= 6.27
+HMX-180°	H= 5.69 O= 4.10	H= 5.56 O= 4.06	H= 8.56 O= 6.73	H= 8.01 O= 6.23
+HMX-270°	H= 5.70 O= 4.07	H= 5.55 O= 3.97	H= 8.58 O= 6.92	H= 7.99 O= 6.31
+DNT-0°	H= 6.38 O= 4.94	H= 4.78 O= 5.72	H= 6.56 O= 8.17	H= 8.36 O= 6.51
+DNT-90°	H= 6.57 O= 4.45	H= 4.15 O= 4.94	H= 8.56 O= 7.21	H= 7.76 O= 7.50
+DNT-180°	H= 6.13 O= 6.76	H= 5.84 O= 3.97	H= 8.55 O= 6.58	H= 7.42 O= 6.81
+DNT-270°	H= 5.11 O= 5.92	H= 5.59 O= 3.74	H= 7.73 O= 7.70	H= 7.31 O= 7.16

Table S2: Calculated currents at 0.05 V for all molecules inside the nanopore.

Tor	***I* (mA)**	***Tor***	***I* (mA)**	***Tor***	***I* (mA)**	***Tor***	***I* (mA)**
+TATP-0°	0.308	+TATP-90°	0.313	+TATP-180°	0.311	+TATP-270°	0.308
+RDX-0°	0.545	+RDX-90°	0.550	+RDX-180°	0.558	+RDX-270°	0.551
+PENT-0°	2.303	+PENT-90°	0.642	+PENT-180°	2.395	+PENT-270°	0.619
+HMX-0°	1.904	+HMX-90°	1.691	+HMX-180°	1.904	+HMX-270°	2.196
+DNT-0°	0.388	+DNT-90°	0.462	+DNT-180°	0.609	+DNT-270°	0.499