Supporting Information: Topology-enabled Quantum Toroidal Moment in Carbon Nanotori

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Supplementary Computational Details

All ground- and excited-state calculations were performed using density functional theory (DFT) and time-dependent DFT (TDDFT) as implemented in Gaussian 16. The M06-2X and CAM-B3LYP exchange–correlation functionals were employed in combination with the 6-31G(d,p) and 6-311++G(d,p) basis sets for systematic comparison. While the 6-31G(d,p) basis provides reliable trends for orbital energies and symmetry classification, the diffuse functions in 6-311++G(d,p) are essential for accurately describing the superatomic molecular orbitals (SAMOs) that extend beyond the carbon cage. The M06-2X functional was chosen following previous benchmarks on C_{60} and related fullerenes, [1] where it reproduces the experimental HOMO–LUMO gap and captures nonlocal exchange effects relevant for delocalized π-systems. CAM-B3LYP, [2] with its range-separated formulation, was employed to verify that excitation characteristics are consistent. Both functionals preserve the qualitative features of the orbital ordering and the toroidal mode composition, confirming that the reported trends are not functional-dependent but intrinsic to the electronic topology of the fullerene tori.

UV-Vis Active and CD Active Excited States of the Carbon Nanotori

We find that for C_{120} in presence of electric field, the CD active states are 41, 42, 52, 55, 78, 94 and 95 with significant rotatory strength (R) values of -2.79, -4.49, -2.14, -1.33, -1.84, -1.87, -3.05 $\times 10^{-40}$ erg esu cm/Gauss, respectively. For C_{144} these states are 25, 26, 65, 66 and 86 with R values of -0.79, -0.92, -0.81, -0.88, -1.04 $\times 10^{-40}$ erg esu cm/Gauss, respectively and for C_{168} the states are 24, 25, 26, 68, 69, 87, 88, 92, 93 with R values of -0.74, -0.82, -0.87, -1.11, -0.95, -0.69, -0.71, -0.83, -1.06 times 10^{-40} erg esu cm/Gauss, respectively. It is important to note that CD-active states and UV-active states do not necessarily coincide, as a transition can have significant oscillator strength without a corresponding rotatory strength, and vice versa.

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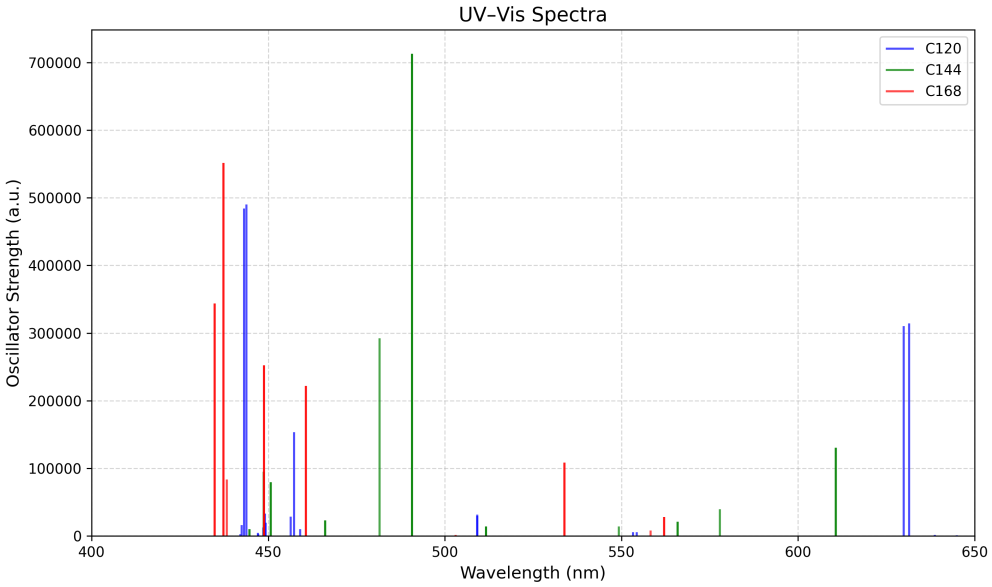

Figure S1: UV–Vis transition spectra of the first 100 excited states of C_{120} (blue), C_{144} (green), and C_{168} (red), computed at the TDDFT level.

Toroidal Projection Results (C$_{168}$ Orbitals) with lesser number of modes

Orbital	**Match (%)**	**Top Modes** (m, n)	**Interpretation**
497	111.25	$(\pm 2, \pm 1)$, $(\pm 5, 0)$, $(\pm 2, \pm 2)$	Mixed toroidal–poloidal
499	96.65	$(\pm 1, \pm 1)$, $(\pm 1, \pm 2)$, $(\pm 1, \pm 3)$	Twisted toroidal
502	79.49	$(\pm 1, \pm 2)$, $(\pm 1, \pm 3)$, $(\pm 1, 0)$	Structured orbital, weak toroidal
503	79.48	$(\pm 1, \pm 2)$, $(\pm 1, \pm 3)$, $(\pm 1, 0)$	Same as 502
504	86.15	$(0, \pm 2)$, $(0, \pm 3)$, $(0, 0)$	Poloidal (cross-sectional)
505	87.21	$(\pm 2, \pm 2)$, $(\pm 2, \pm 3)$, $(\pm 2, \pm 4)$	Mixed, nodal structure
506	87.21	$(\pm 2, \pm 2)$, $(\pm 2, \pm 3)$, $(\pm 2, \pm 4)$	Same as 505
507	8.51	$(\pm 1, \pm 1)$, $(\pm 1, \pm 2)$, $(\pm 1, \pm 3)$	Weak overlap, non-toroidal
508	8.51	$(\pm 1, \pm 1)$, $(\pm 1, \pm 2)$, $(\pm 1, \pm 3)$	Same as 507
509	88.90	$(0, \pm 1)$, $(0, \pm 2)$, $(0, \pm 3)$	Strongly poloidal
510	26.77	$(\pm 1, \pm 2)$, $(\pm 1, \pm 1)$, $(\pm 1, \pm 3)$	Structured orbital, weak character
514	88.87	$(0, \pm 1)$, $(0, \pm 2)$, $(0, \pm 3)$	Strongly poloidal
515	88.88	$(0, \pm 1)$, $(0, \pm 2)$, $(0, \pm 3)$	Same as 514

Table S1: Toroidal character summary for C$_{168}$ molecular orbitals ($R = 6.22$ Å, $r = 1.83$ Å, $m, n \leq 5$). A dashed line is used to separate the filled and vacant orbitals.

References

[1] Arkamita Bandyopadhyay and Jamal Berakdar. Magnetic properties and spin–spin interaction in nitrogen-doped fullerene nanostructures. *The Journal of Chemical Physics*, 163(1):014308, 07 2025.

[2] Takeshi Yanai, David P Tew, and Nicholas C Handy. A new hybrid exchange–correlation functional using the coulomb-attenuating method (cam-b3lyp). *Chemical Physics Letters*, 393(1):51–57, 2004.