

Cite this: DOI: 00.0000/xxxxxxxxxx

Electronic Supporting Information (ESI)

Magnetic response properties of carbon nano-onions

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Received Date

Accepted Date

DOI: 00.0000/xxxxxxxxxx

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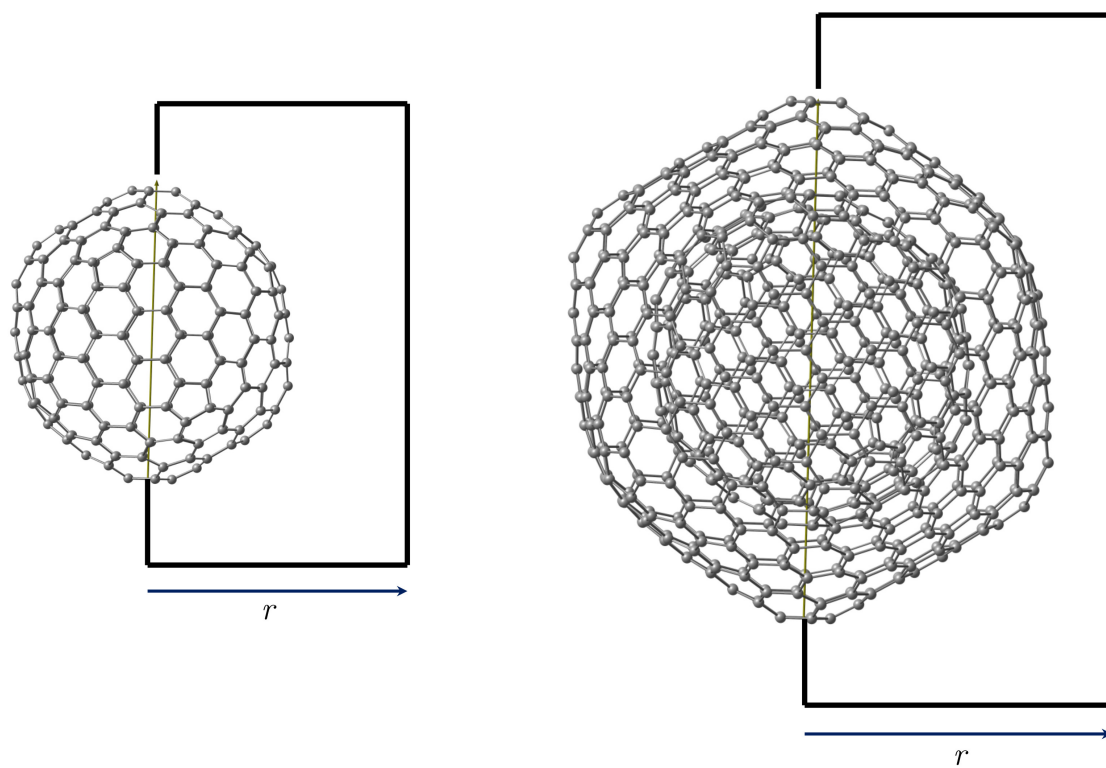


Fig. S1 Schematic of the integration planes used in this work for single-layer fullerenes (left) and C_n -CNOs (right). The height of these planes measured from the bottom to the top is 30 Å, while the radial width extends to 15 Å. The structures were oriented with the z axis (shown with a yellow arrow) perpendicular to a 5- or 6-MR as appropriate. The r coordinate of the ring-current strength profiles runs on the horizontal axis of these planes.

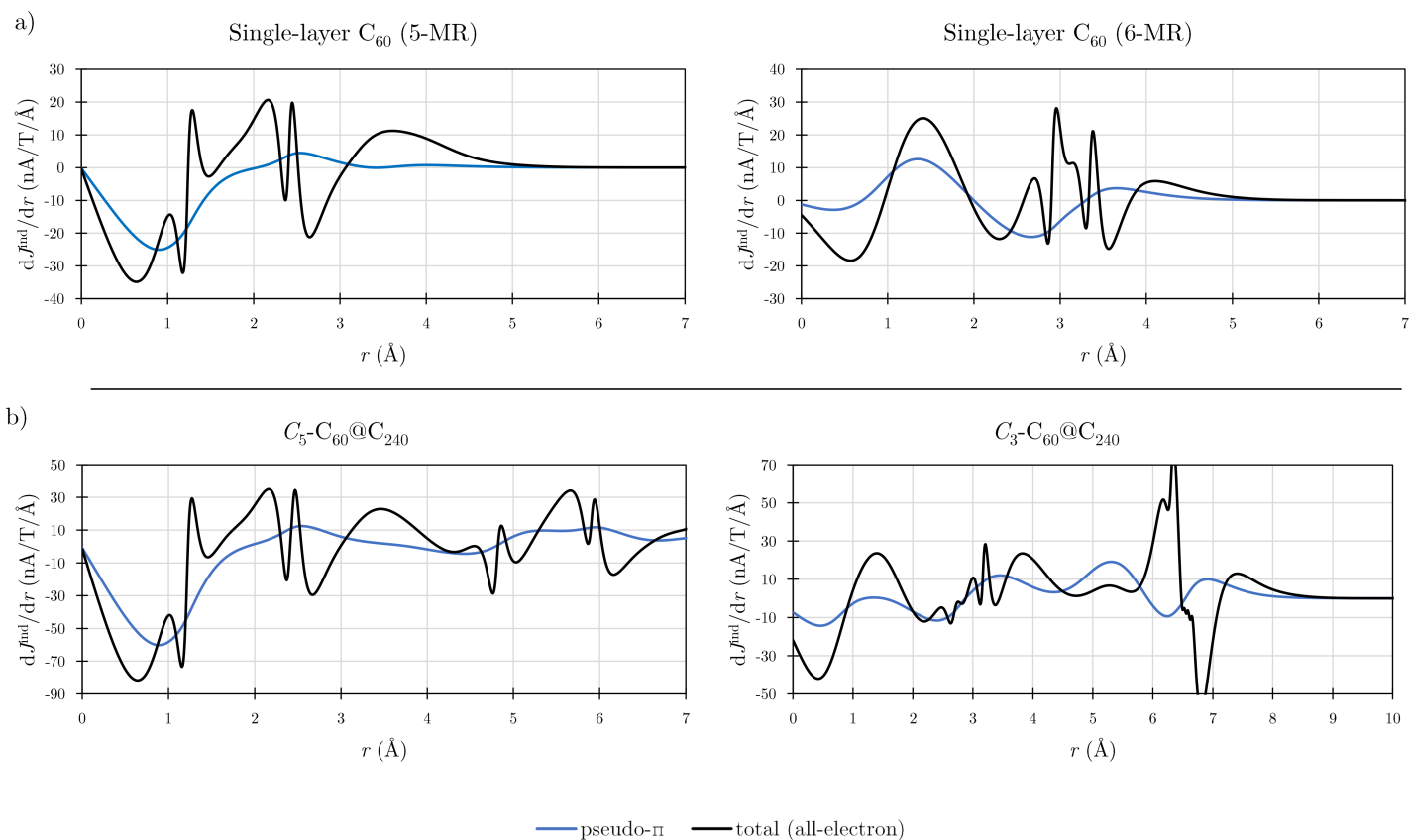


Fig. S2 The pseudo- π and total (all-electron) ring-current strength profiles (dJ^{ind}/dr) for a) single-layer C_{60} and b) C_n - $C_{60}@C_{240}$ corresponding to the cases when \mathbf{B}^{ext} is perpendicular to common inter-layer 5-MRs (and 6-MRs), calculated at the CAM-B3LYP/def2-SVP level. The total and pseudo- π ring-current strength for C_{60} is -12.0 (6.32) and -22.2 (2.37) nA/T, respectively. The total and pseudo- π ring-current strength for C_n - $C_{60}@C_{240}$ is -17.84 (21.56) and -31.9 (13.8) nA/T, respectively.

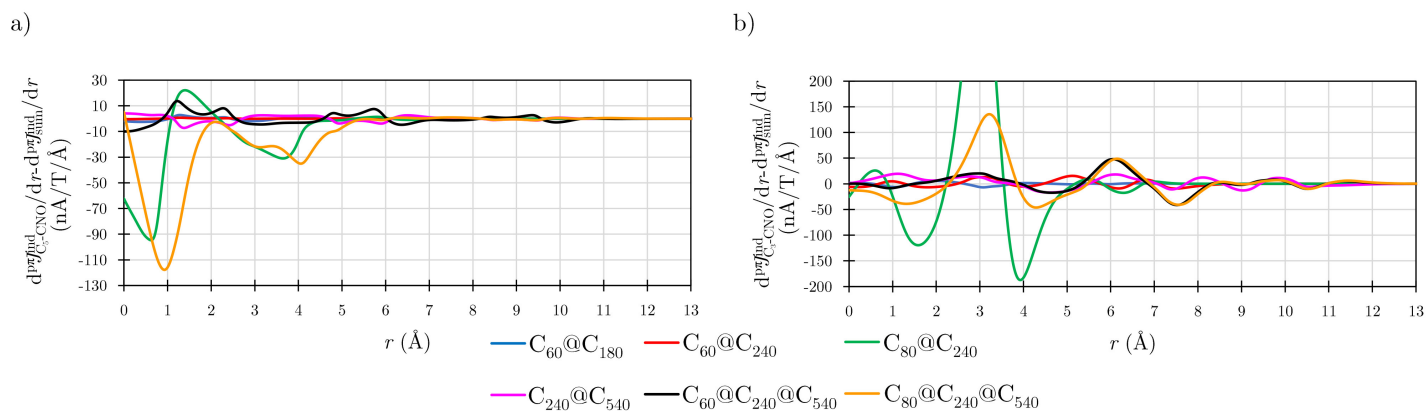


Fig. S3 The pseudo- π ring-current strength profiles of the differences resulting from subtracting the profile of the sum of its single-layer components ($d^{pseudo-\pi} J_{sum}^{ind}/dr$) from profile of a) C_5 -CNOs ($d^{pseudo-\pi} J_{C_5-CNO}^{ind}/dr$) and of b) C_3 -CNOs ($d^{pseudo-\pi} J_{C_3-CNO}^{ind}/dr$) corresponding to the cases when \mathbf{B}^{ext} is perpendicular to common inter-layer 5-MRs and 6-MRs, respectively, calculated at the CAM-B3LYP/def2-SVP level.