

Supporting Information:

**Magnetically Induced Ring-Current Strengths of Planar
and Nonplanar Molecules: New Insights from The Pseudo-
 π Model**

Mesías Orozco-Ic,^{*,†} Maria Dimitrova,[‡] Jorge Barroso,[†] Dage Sundholm,^{*,‡} and Gabriel Merino,^{*,†}

[†]*Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados, Unidad Mérida. Km 6 Antigua Carretera a Progreso. Apdo. Postal 73, Cordemex, 97310, Mérida, Yuc., México.*

[‡]*Department of Chemistry, Faculty of Science, University of Helsinki, P.O. Box 55, A. I. Virtasen aukio 1, FIN-00014 Helsinki, Finland.*

Corresponding Authors

*E-mail: mesias.orozco@cinvestav.mx (M.O.-I.).

*E-mail: dage.sundholm@helsinki.fi (D.S.)

*E-mail: gmerino@cinvestav.mx (G.M.)

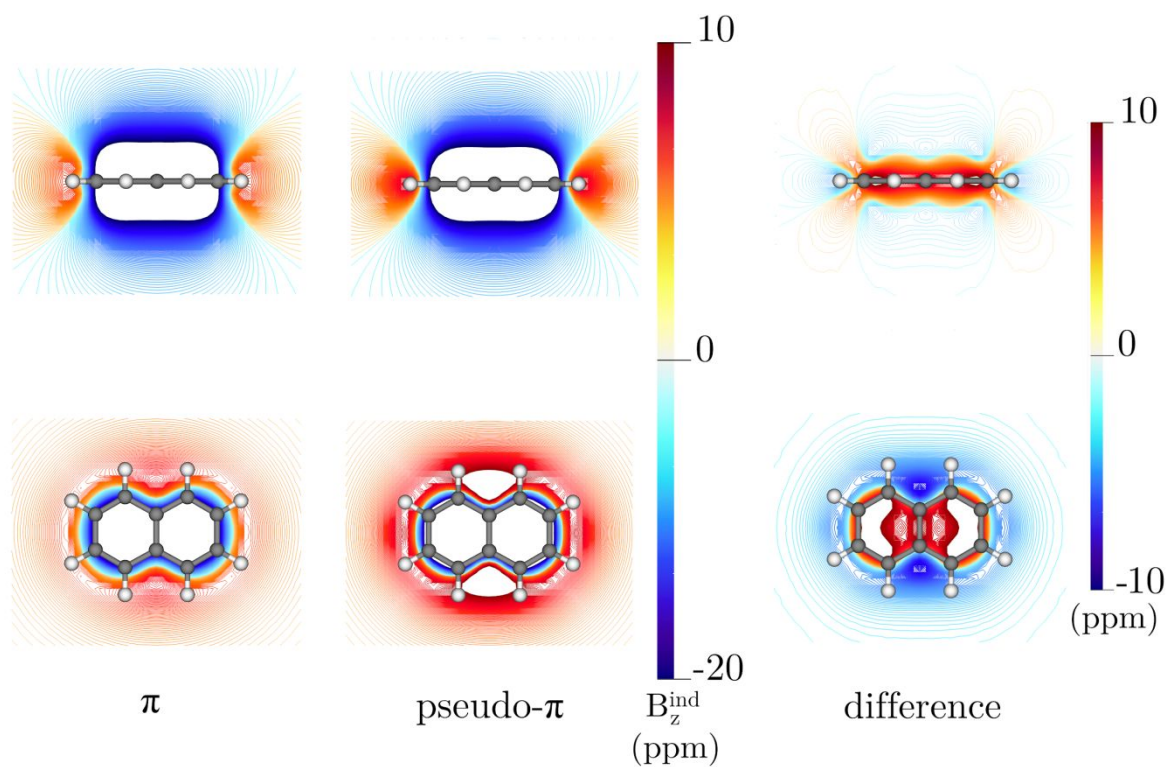


Figure S1. Comparison of the true π -component of B_z^{ind} (left), the pseudo- π modeled (in the middle), and the difference resulting from subtracting the pseudo- π model computations from the true π -component computed in the same grid (right) for naphthalene. The true π -component can be computed using the Nuclear Chemical Shielding (NCS) analysis, which allows to dissect the shielding tensor into its molecular orbital components.

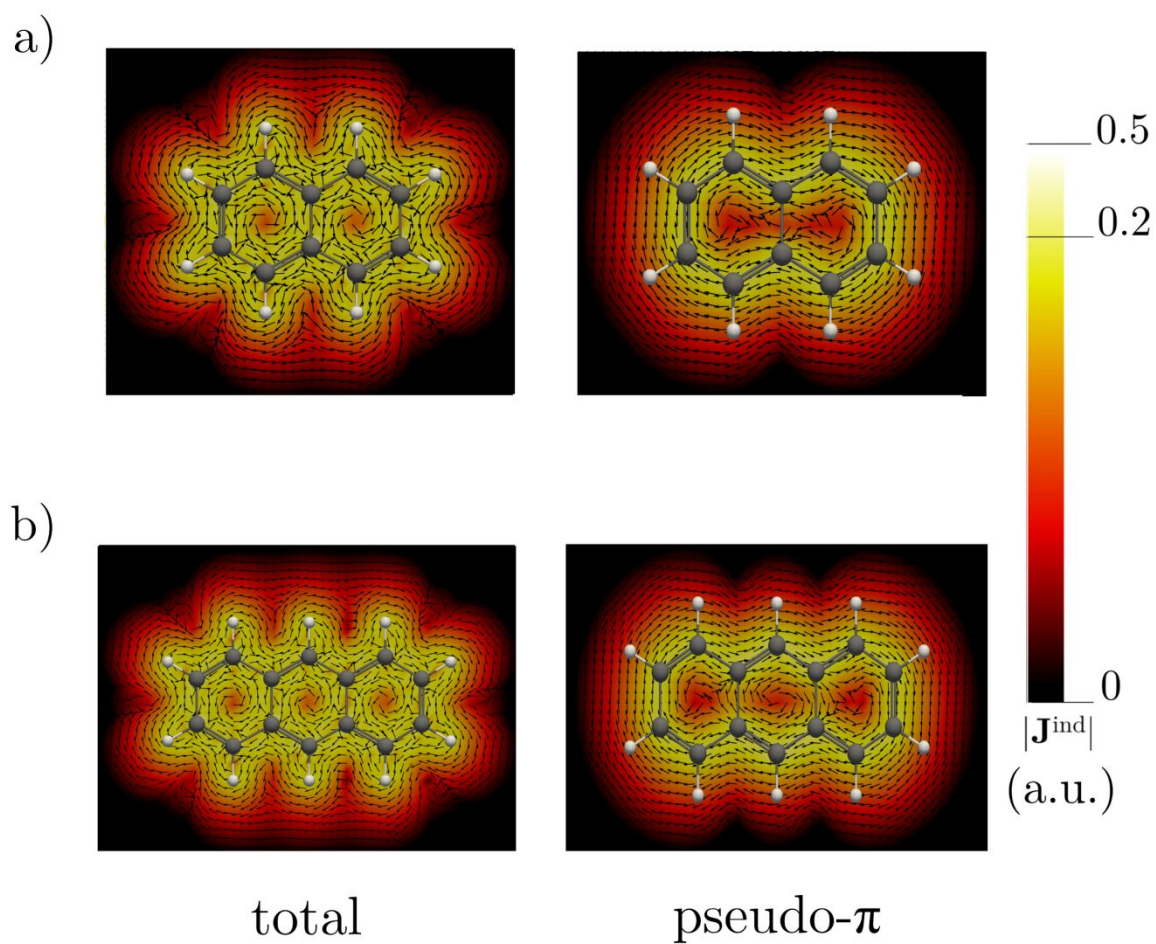


Figure S2. The total \mathbf{J}^{ind} (left) and the pseudo- π contribution to \mathbf{J}^{ind} (right) computed in the molecular plane of a) naphthalene and b) anthracene. The arrows show the direction of the current density. The $|\mathbf{J}^{\text{ind}}|$ scale is given in atomic units (1 a.u. = 100.63 nA/T/Å²).

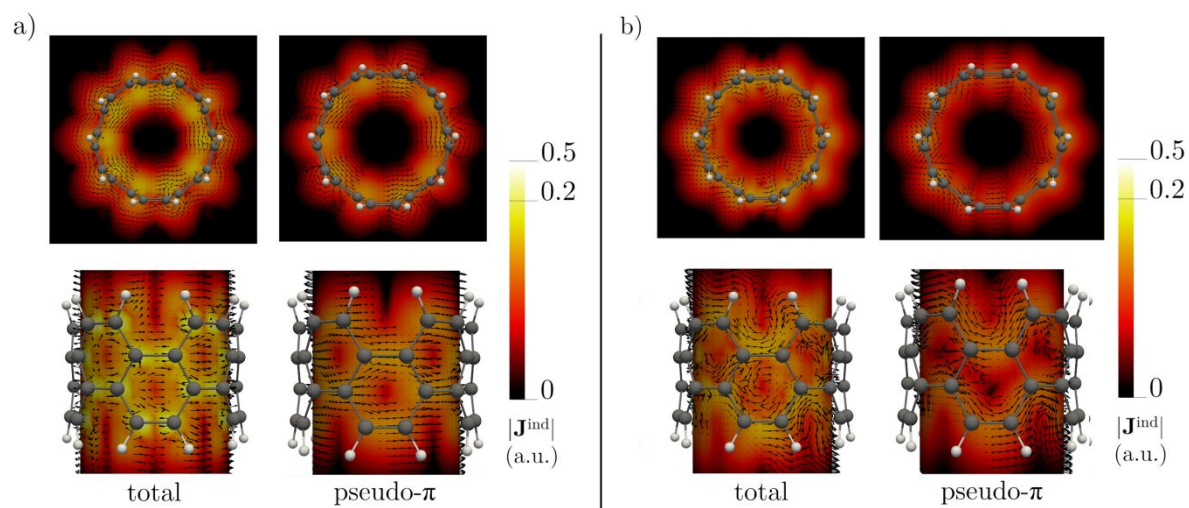


Figure S3. a) The total (left) and the pseudo- π modeled (right) \mathbf{J}^{ind} computed in a perpendicular plane (top) to the external field and in a cylindrical plane (bottom) for [10]cyclophenacene. The external field is parallel to the belt axis (z -axis). b) The total (left) and the pseudo- π modeled (right) \mathbf{J}^{ind} calculated in a perpendicular plane (top) to the external field and in a cylindrical plane (bottom) for [10]cyclophenacene. The external field is perpendicular to the belt axis (y -axis). The arrows show the direction of the current density. The $|\mathbf{J}^{\text{ind}}|$ scale is given in atomic units (1 a.u. = 100.63 nA/T/Å²).

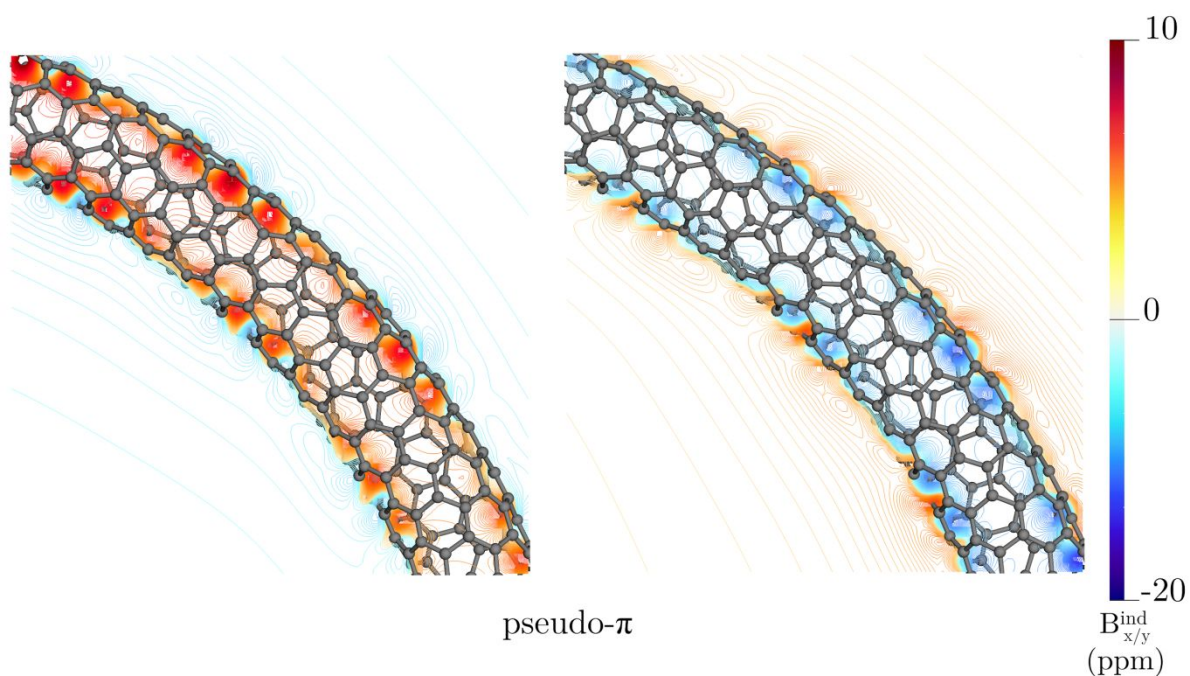


Figure S4. Isosurfaces of the x - (left) and y -component (right) of the induced magnetic field using the pseudo- π model computed in a molecular plane for C_{2016} . The magnetic field is parallel to the toroidal axis.

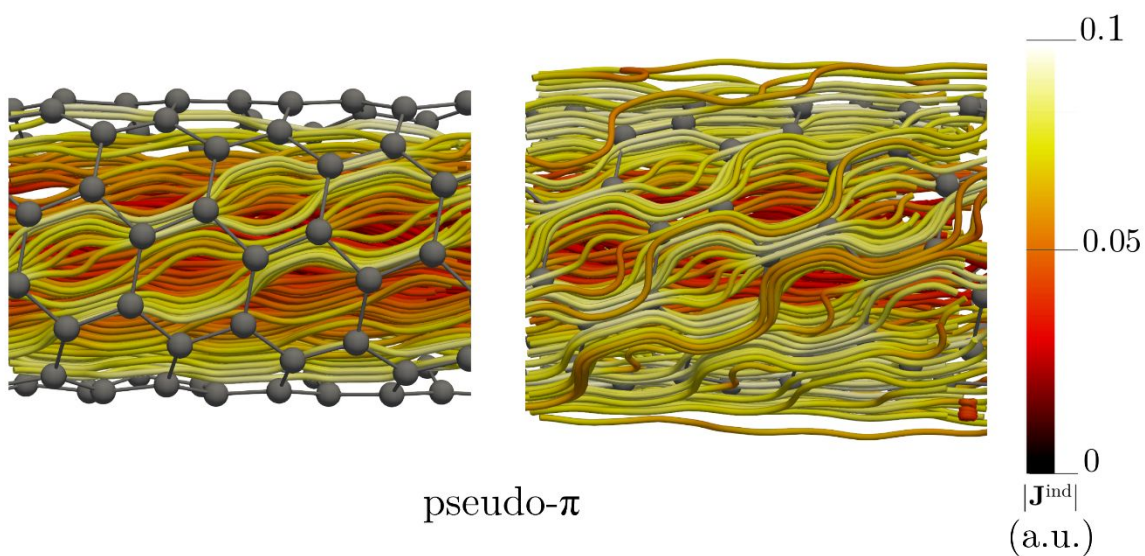


Figure S5. Streamlines representation of \mathbf{J}^{ind} showing the currents pathways flowing diatropically outside (left) and inside (right) of the surface of the toroidal carbon nanotube (C_{2196}) using the pseudo- π model. The external field is parallel to the main axis of the torus.

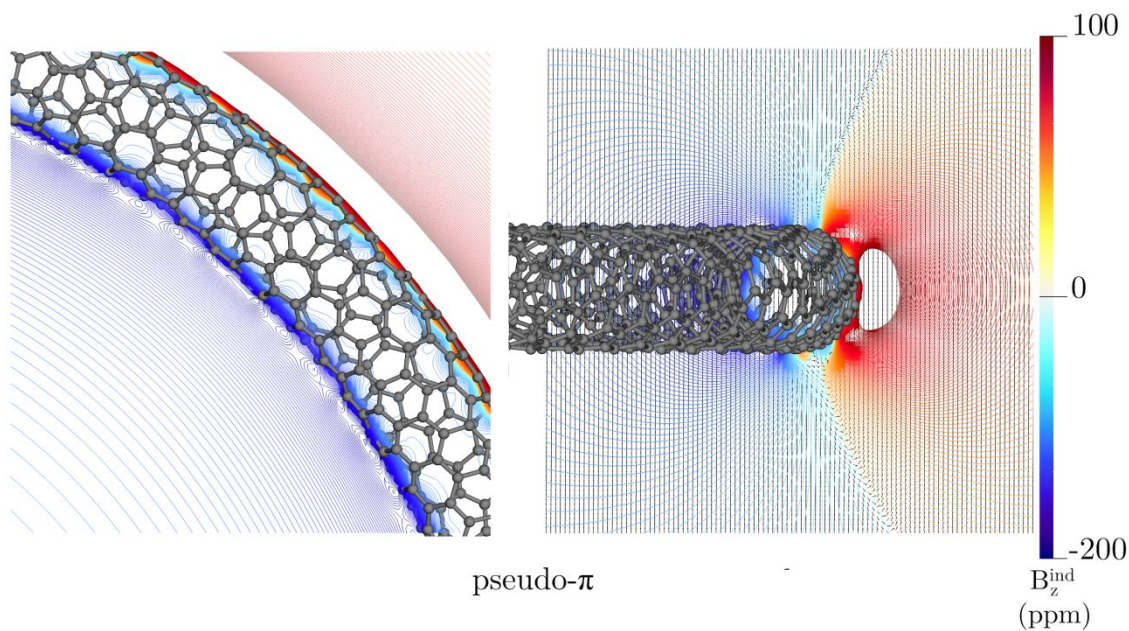


Figure S6. The induced magnetic field (\mathbf{B}^{ind}) computed with the pseudo- π model (right) in a molecular plane (left) and a perpendicular plane (right) for C_{2196} . The arrows show the direction of \mathbf{B}^{ind} , while the color scale denotes the strength of the z -component of the magnetic field. The magnetic field is parallel to the toroidal axis.