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Magnetic response properties computed with the pseudo-π model, from molecules to nanostructures.

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Content

The pseudo-π model yields current densities and induced magnetic fields that mimic the π-component, allowing investigations of large molecular structures, whether they are planar or not, at a low computational cost but with high accuracy. Herein the π-contribution to the magnetically induced current densities and induced magnetic fields of large planar molecules and nonplanar molecules (were computed using the pseudo-π model with the gauge-including magnetically induced currents method. [1-4] Additionally, we provide a way to determine the π-component of the ring-current strengths, which can be used for assessing the aromatic (or antiaromatic) character of large carbon molecules.

References [1] Mesías Orozco-Ic, M. Dimitrova, J. Barroso, D. Sundholm, G. Merino. J. Phys. Chem. A. 2021, 125, 5753-5764. [2] Mesías Orozco-Ic, R. R. Valiev, D. Sundholm. Phys. Chem. Chem. Phys. 2022, 24, 6404-6409. [3] Mesías Orozco-Ic, D. Sundholm. Phys. Chem. Chem. Phys. 2022, 24, 22487-22496. [4] Mesías Orozco-Ic, L. Soriano-Agueda, S. Escayola, D. Sundholm, G. Merino, E. Matito. J. Org. Chem. 2024, 89, 2459-2466.

Tipo de presentación

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Primary author(s) : Dr. OROZCO-IC, Mesias (Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca 62210, México.)

Presenter(s) : Dr. OROZCO-IC, Mesias (Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca 62210, México.)