

Magnetically-induced current density investigation in carbohelicenes and azahelicenes

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In this poster, we investigate the magnetically-induced current (MIC) density for a variety of ortho fused polycyclic aromatic molecules at the density functional theory level with the gauge including magnetically induced current (GIMIC) method (Figure 1). With this method, the aromatic character of each ring in a homologous series of carbohelicenes with an increasing number of fused benzene rings is assessed and compared with other aromaticity criteria such as Nucleus Independent Chemical Shifts [NICS(0), NICS_{zz}(0)] and Bond Length Alternation (BLA) parameters. All criteria indicate that the two outer rings are the most aromatic ones [*i.e.* higher induced current, more negative NICS(0) and NICS_{zz}(0) values, and smaller BLA values]. For the large helicenes ($n > 10$), the current drops along the following four rings and then rise again. Additionally, we have proven that this behavior is not due to a difference of the local magnetic field coming from a difference of orientation of the ring with respect to the external magnetic field (oriented along the helical axis). Upon fusing additional benzene rings to form the hexa-peri-hexabenz[7]helicene, some rings (B, D, and F) are a lot less aromatic (even non-aromatic) than the others. The NICS(0) and NICS_{zz}(0) values exaggerate this behavior because they are all positive values, which is a signature of antiaromaticity. Then, when substituting one, three, or four benzene rings by pyrrole ones to form the mono-aza-[7]-helicene, the triaza-[7]-helicene, and the tetra-aza-[7]-helicene, remarkable changes in the electronic structures of helicenes are observed. Indeed, the induced currents are always smaller in the pyrrole rings than in the benzene ones.

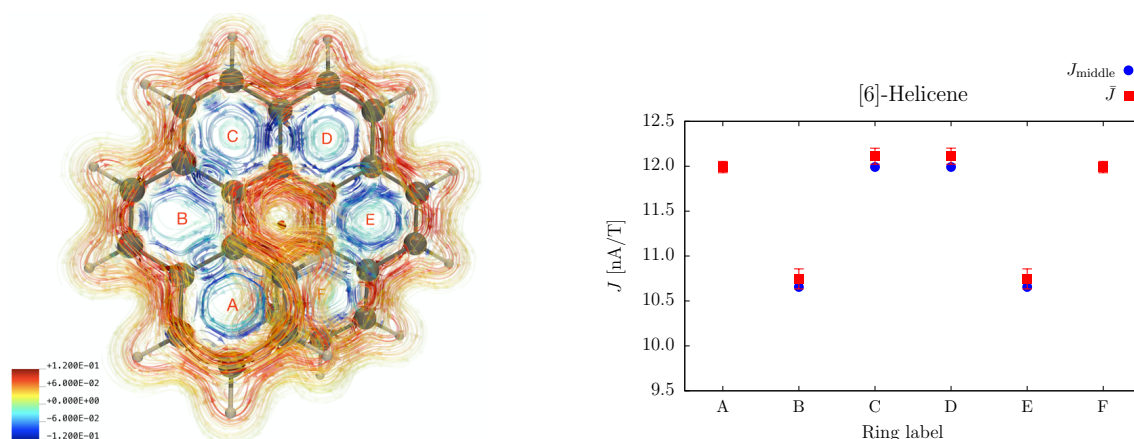


Figure 1: 3D Streamline plot of the current density (left) and total induced current (right) for [6]-helicene molecules.

References

1. Emna CHERNI, Benoît CHAMPAGNE, Sameh AYADI and Vincent LIÉGEOIS, *Phys. Chem. Chem. Phys.* (2019) DOI: 10.1039/c9cp02071c.