Switch from local to global aromatic character in Möbius carbon nanobelts upon dioxidation. Evaluation of magnetic behavior in neutral and charged species

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Abstract

Here we show that recent Möbius carbon nanobelts (MCNBs) can be switched from a local to a global aromatic behavior upon dioxidation. Hence, large aromatic structures can be achieved by the choice of the charge states, giving rise to shielding cone characteristics extended within the overall structure at the nanoscale regime, pushing the limit of aromatic circuits to 198 π-electrons.