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Cilindrična aromatičnost u ferocenu i njegovim analozima

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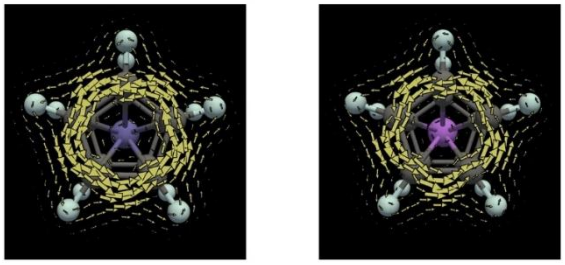
Još od otkrića ferocena, aromatični karakter ovog molekula bio je predmet mnogih istraživanja. U ovom radu, aromatičnost ferocena i njegovih analoga analizirana je primenom modela čestice u cilindru. Naime, rešenja Šredingerove jednačine za česticu koja se kreće u cilindru su funkcije koje se razlikuju po broju i prirodi nodalnih površina. Nađeno je da se molekulske orbitale ispitivanih molekula mogu povezati sa sopstvenim funkcijama modela čestice u cilindru. Gustine magnetno indukovanih struja su izračunate primenom CTOCD-DZ metode na B3LYP/LANL2DZ nivou teorije za svaku od podgrupa molekulskih orbitala. Pokazano je da popunjenost dobijenih podgrupa molekulskih orbitala u ferocenu prati Hikelovo 4n+2 pravilo.



Slika 1. Mape gustine struja za $C_{10}H_{10}Fe$ i $C_{10}H_{10}Li^-$.

Cylindrical aromaticity in ferrocene and its analogues

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The aromatic character of ferrocene has been extensively investigated since its discovery. In this work the aromaticity of ferrocene and its analogues was rationalized by the hollow cylinder model. Solving the Schrödinger equation for a particle in the hollow cylinder model gives eigenfunctions which can be classified based on their nodal characteristics. It was found that the molecular orbitals of the studied molecules follow the nodal properties of the eigenvectors of the simple cylinder model. Magnetically induced current densities were calculated using the CTOCD-DZ method at the B3LYP/LANL2DZ level of theory for each molecular orbital subgroup. It was found that populations of the orbital subgroups follow the Hückel 4n+2 rule.

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