Understanding Aromaticity and Antiaromaticity with Information-Theoretic Approach in Density Functional Theory

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Originated from the cyclic delocalization of electrons resulting in extra stability and instability, aromaticity and antiaromaticity are important chemical concepts whose appreciation and quantification are still much of recent interest in the literature. Employing informationtheoretic approach quantities can provide us with more insights and better understanding about them, as we will demonstrate in this work. We examine the ground state, triplet-state, and macrocyclic aromaticity and antiaromaticity, which are governed by Hückel's 4*n* + 2 rule, Baird's 4*n* rule, and Mobius 4*n* rule, respectively, for a number of different species. We analyze the numerical results using total energy partition schemes and information-theoretic approach in density functional theory. We also compare our results with conventional aromaticity indices from the literature. Strong linear correlations of molecular property descriptors with aromaticity indices enable us to better understand the nature and propensity of aromaticity and antiaromaticity for these systems. Our results not only illustrate the existence and validity of various circumstances and propensities governed by different aromaticity and
antiaromaticity rules, but also show that Hückel, Baird, Mobius and other rules might share the same theoretical origin. These results should provide new insights into the nature of aromaticity and antiaromaticity in different situations and pave the road toward new ways to quantify aromaticity and antiaromaticity, an extremely important pair of chemical concepts.

References:

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