

Aromaticity: Past, Present and Future

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Aromaticity, one of the most fundamental concepts in chemistry, has attracted considerable attention from both theoreticians and experimentalists. However, besides metallabenzenes, other transition metal-involved aromatics are less developed. Here, we report the important role of transition metals in several metallaaromatics by density functional theory calculations. Specifically, Craig-type Möbius aromaticity,^[1-2] σ -aromaticity dominating in an unsaturated ring,^[3] hyperconjugative aromaticity^[4] and adaptive aromaticity^[5] are achieved due to an introduction of transition metals.^[6] All these findings show a magic power of transition metals originating from participation of more electrons from *d* orbitals in aromaticity rather than one electron for the carbon atom, opening an avenue to the design of novel metalla-aromatics. Finally, the application of aromaticity in N₂ activation will be also discussed.^[7]

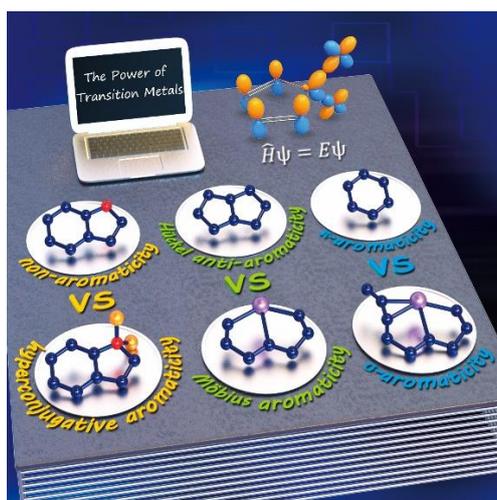


Figure 1. Schematic illustration of some unconventional aromaticities

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