Aromaticity: Past, Present and Future

Jun Zhu*

Department of Chemistry, Xiamen University, Xiamen, P.R. China, 361005

jun.zhu@xmu.edu.cn

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 rule of transition metals in several metallaaromatics by density functional theory calculations. Specifically, Craig-type Möbius aromaticity,[1-2] -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 N_2 activation will be also discussed.[7]

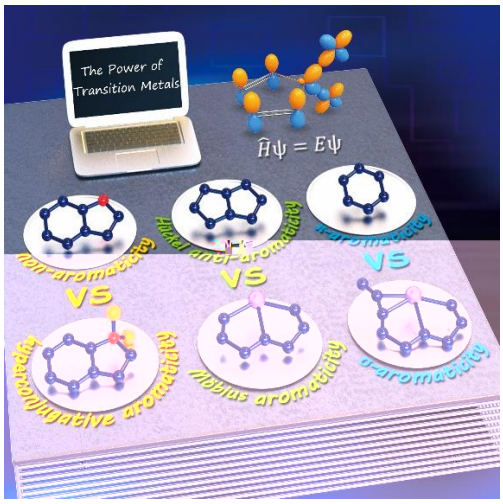

Figure 1. Schematic illustration of some unconventional aromaticities

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