MULTIPLE AROMATICITY, CONFLICTING AROMATICITY AND MULTIPLE ANTIAROMATICITY IN CLUSTERS

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Currently there is no simple chemical bonding model allowing us to use the “paper and pencil” approach for predicting global minima and low-lying isomers of homoatomic and heteroatomic clusters. However some progress in developing such a model has been made in recent years. In order to facilitate this process we recently developed a new theoretical tool for analysis of wave functions – Adaptive Natural Density Partitioning analysis (AdNDP). Unlike conventional Natural Bond Analysis, AdNDP is capable of identifying multicenter (with number of centers equal to or less than the total number of atoms in the system) two electron bonds in addition to lone pairs and two center – two electron localized bonds. In the current presentation we demonstrate how from joint theoretical and experimental study of clusters and using our AdNDP analysis we can explain and predict structure, stability and other molecular properties of clusters using multiple ($\sigma$, $\pi$, $\delta$, $\phi$) aromaticity, conflicting aromaticity (simultaneous presence of aromaticity and antiaromaticity), or ($\sigma$, $\pi$, $\delta$, $\phi$) multiple antiaromaticity. Boron, aluminum, carbon-boron, doped aluminum, and other main group and transition metal clusters, will be used as examples.

References