



Electron Density Analysis Tools

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Message from the Guest Editor

Modern electron density analysis methods are powerful tools for obtaining chemical insight from quantum chemical calculations. At least two kinds of different approaches can be distinguished: (i) Real space methods, sometimes grouped within the term of quantum chemical topology and comprising, among others, Bader's quantum theory of atoms in molecules (QTAIM) or the topological study of the electron localization function (ELF); and (ii) those methods where orbitals are still considered as significant mathematical entities, natural bonding orbital (NBO) probably being the most widely used. Extensive application of these techniques on several chemical topics has enriched our knowledge on the electronic origin of diverse physical and chemical properties, trends, or concepts. In many cases, electron density analysis has provided conclusions that are fully compatible with firmly rooted ideas within the chemical community. This Special Issue focuses on recent advances in methods, implementations for analyzing specific properties or systems, extensions of already developed methods, and significant applications of electron density analysis tools.





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Message from the Editor-in-Chief

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