Special Issue

Electron Density Analysis Tools

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.

Guest Editor

Prof. Dr. Ricardo Mosquera
Department of Physical Chemistry, Universidad de Vigo, Vigo, Spain

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Molecules
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
molecules@mdpi.com

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Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt
Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

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