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Electron Density Distribution in Crystals: New Results in Understanding the Nature of Chemical Bonding.

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New approaches and results in the experimental electron density distribution (EDD) analysis in molecular crystals using X-ray diffraction method will be presented together with high-quality quantum-chemical calculations of the peculiarities of chemical bonds of different types in the series of different compounds.

New approaches are based on a wide application of modern multipole model for an analytical presentation of the EDD and its characteristics, topological analysis of the EDD function, analysis of the electron localization function and estimation of the energetic characteristics of inter-atomic interactions (potential and kinetic energy densities) directly from X-ray diffraction data. As examples of the compounds studied the EDD, features of chemical bonding and electronic structure of different compounds will be critically analyzed (atranes, including boratranes, silatranes, carboranes and metallacarboranes, metallocenes and their derivatives, para-cyclophanes, crystals with strong hydrogen bonds, organic high-energy and non-linear optical materials. The data obtained allowed one to formulate some new ideas about chemical bonding in these compounds and estimate in some cases their important properties from X-ray diffraction data only.