ELF characterization of I-I/S-I bonds in polyiodides

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The range of iodine-iodine and sulphur-iodine chemical bonds in polyiodides with organic compounds are the subjects of researcher`s interest both from theoretical and experimental crystal engineering. Discrete, chain, net polyiodides, iodonium derivatives with S-I^+-S fragment and molecular complexes with strongly bound diiodine S…I-I are considered within the framework of ELF distribution in crystals and validated by the experimental and calculated Raman data.[1] The features of ELF redistribution in the region within polyiodide anions were found. ELF values in bond critical points of electron density for I-I/I…I bonds are more reliable in characterization of bound I_2 inside polyiodide anions than analysis of bond lengths. Consistent usage of experimental and theoretical methods can reveal the bound iodine inside polyiodide anions of complex structure and predict characteristic features of such crystals, such as low thermal stability and iodine loss under heating[2].

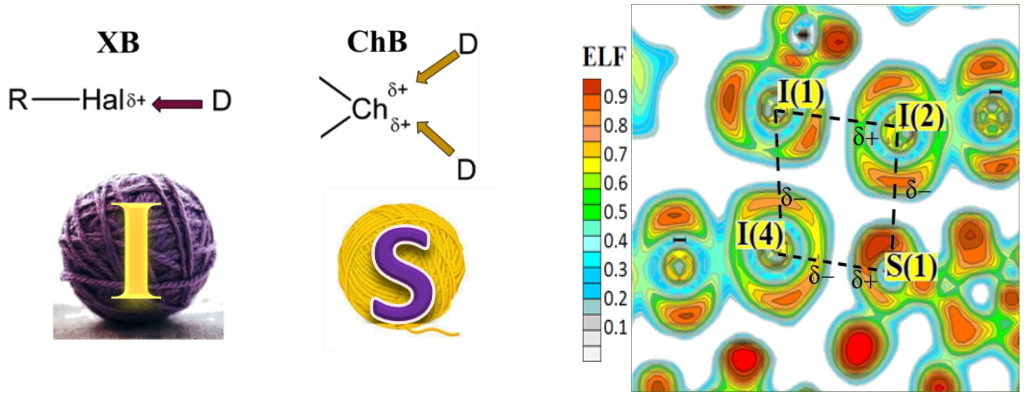

Figure 1 The net of halogen and chalcogen I...I and I...S interactions in ELF representation of benzoxazolothiazinium triiodide

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[1] Savin A. J. Phys. Chem. Solids, 2004
[2] Bartashevich E.V., Mukhitdinova S.E., Yushina I.D., Tsirelson V.G. Acta Crystallogr. B, 2019