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New models of electron density for electrostatic interaction energy estimation

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The accurate estimation of electrostatic interaction energies in a reasonable time is a still challenging task. The simple summation of multipole moments is fast, but it does not account the penetration energy (Epen). The Epen can be up to 50% of total electrostatic interaction energy (Ees) at the equilibrium distance.

Our concept is taken from the theoretical crystallography. We applied aspherical pseudoatom databank (University at Buffalo DataBank - UBDB) which can easily reproduce the averaged electron density and calculate the Ees. We also tested reproduced electron densities from a new algorithm of refinement procedure, which differs from this commonly used in the databanks. However, the best performance is achieved when the promolecule model of an electron density is augmented by point charges fitted to electrostatic potential (RESP). It enables estimation of the exact electrostatic interaction energy and, by its simplicity, it allows to omit computational-costly integration procedure. Our recent researches show that the RESP charges can be successfully replaced by the point charges from other - easy attainable - sources: from database or from semiempirical methods.

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'Pancake' bonding: a charge density perspective

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A class of thiazyl radicals, 1,2,3,5-dithiadiazolyls (R-CNSSN•, hereafter DTDAs), have been the focus of much investigation due to their potential as building blocks for magnetic and conducting materials. [1] However, these molecules tend to dimerise in the solid state *via* a spin-pairing interaction known as 'pancake bonding' [2], rendering them diamagnetic. Experimental charge density analysis has been carried out on a number of DTDA homodimers, heterodimers and monomers. [3] These data, as well as various computational results, are assessed to probe the nature of the 'pancake bonds' in DTDAs.

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