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A novel definition of a molecule in a crystal

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Abstract

A new method for dividing a crystalline electron distribution into molecular fragments is proposed, based on Hirshfeld's partitioning scheme. Unlike other approaches, the method partitions the crystal into smooth molecular volumes as well as intermolecular voids of low electron density. To compare the new method with several other schemes which subdivide a crystal into molecules, numerical integration is performed on two model electron densities (one representing a superposition of isolated molecules, the other interacting molecules) for ice VIII, formamide and urea. The new scheme is simply to apply, aesthetically appealing, and offers some promise in routine partitioning of crystalline electron densities or in computer graphics to provide additional insight into molecular packing in crystals.

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