Electron number probability distributions in crystals

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Any region coming from an arbitrary partition of the space has a certain probability of being occupied by an exactly integer number of electrons. The probability of such an event can up to now be computed for single- [1] and multi-determinant [2] wave functions in molecules. An extension of this work to crystals is presented here, together with some examples for simple model systems using the Quantum Theory of Atoms In Molecules (QTAIM) partitioning. Our results show that domain probabilities in solids might become an interesting new tool to examine chemical bonding in extended systems.

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[2] FRANCISCO, E.; PENDÁS, A. Martín; BLANCO, M. A. Electron number probability distributions for correlated wave functions. The Journal of chemical physics, 2007, 126. Jg., Nr. 9, S. 094102.