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The Partition Problem; Insights from Density Functional Theory

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How to partition a system into its components, the atoms in molecules problem and its multi-atomic generalizations, arises ubiquitously in physics, chemistry, and materials science. It is central to population analysis, chemical reactivity theory, issues of transferability, and relevant to computational methods for very large systems such as QM-MM and O(N) schemes. At issue is the decomposition of the total electron density into contributions from each part, whence the relevance of density functional theory. My collaborators and I have developed a new, exact scheme, partition theory, for that decomposition. It is based on the Perdew, Parr, Levy, and Balduz ensemble formulation of density functional theory. In this talk, the elements of partition theory will be described, including its formal structure, a dynamical version for efficient computation, and quantitative illustrations of its central features via the partition of very simple systems.