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Partition Density Functional Theory

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Partition Density Functional Theory (PDFT) is a formally exact method for obtaining molecular properties from self-consistent calculations on isolated fragments [1,2]. For a given choice of fragmentation, PDFT outputs the (in principle exact) molecular energy and density, as well as fragment densities that sum to the correct molecular density. I describe our progress understanding the behavior of the fragment energies as a function of fragment occupations, derivative discontinuities, practical implementation, and applications of PDFT to small molecules. I also discuss implications for ground-state Density Functional Theory, such as the promise of PDFT to circumvent the delocalization error of approximate density functionals.

[1] M.H. Cohen and A. Wasserman, J. Phys. Chem. A, 111, 2229(2007).
[2] P. Elliott, K. Burke, M.H. Cohen, and A. Wasserman, Phys. Rev. A 82, 024501 (2010).