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Recent Developments in Fragment-based Density Functional Theory

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I describe our progress on the development, implementation, and application of partition density functional theory (PDFT), a formally exact method for obtaining molecular properties from self-consistent calculations on isolated fragments [1]. 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 discuss the behavior of the fragment energies as a function of fragment occupations [2], the different ways in which PDFT can be used to avoid the delocalization and static-correlation errors of approximate density functionals [3], our recent extension to the time-dependent case [4], and future directions.

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[3] J. Nafziger and A. Wasserman, arXiv:1305.4966
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