

# Two-Point Weighted Density Approximations for the Kinetic Energy and Exchange-Correlation Energy

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Many of the problems in density-functional theory can be mitigated by carefully designing an exchange-correlation hole with the proper mathematical properties. This leads to generalized and extended versions of the venerable weighted density approximation (WDA). In this talk, I will show how well WDA can work for the kinetic energy, exchange energy, and exchange-correlation energy. One advantageous feature of the WDA is that it allows one to deal with fractionally occupied sites in a better way than conventional functionals. (For example, the H<sub>2</sub> dissociation problem is entirely solved.) The traditional criticism of WDA has been its high computational cost. These costs are mitigated by new algorithms using a new limited-memory quasi-Newton method that was designed especially for this application.