Locally Parameterized Exchange and Correlation Functionals. Can a non-empirical GGA describe accurately finite and extended systems?

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To date it has not been possible to design a non-empirical approximate exchange and correlation (XC) functional with general applicability. Simple functionals (dependent on the density and low-order spatial derivatives) that work well for molecules do poorly on solids and conversely. Functionals that include exact-exchange need different fractional contributions for different system classes and are computationally costly for large complicated systems. In this talk a non-separable, non-empirical generalized gradient approximation (GGA) XC functional, aiming to balanced application in both finite (atoms and molecules) and extended systems (solids) is proposed. The central idea is to propose that the parameters appearing in a standard separable GGA X functional should in fact depend on the electron density. Such locally parameterized (*lp*) functionals are constructed by connecting the coefficients corresponding to the gradient of the density in what originally was the C contribution with those in what originally was the X contribution. The connection is made by imposing the condition that the two contributions cancel, thereby recovering the linear response of the uniform electron gas. Associating the low-density limit with uniform electron gas exchange and the high-density limit with the value obtained by Ma and Brueckner (as used to fix the value of the exchange coefficient in the PBE GGA) one obtains the *lp* functionals. The advantage is that *lp* functionals have the capability of tuning the quadratic contribution to the exchange-like term between the two density limits without requiring dependence upon the density laplacian or the kinetic energy density. Because of the density-dependent parameters, the contributions no longer scale as pure X or pure C, hence the non-separability. The validation and application of these DFAs is presented, paying special attention to magnetic behavior of pure transition metals and CO physisorption on some surfaces of transition metals.