# Density-functional theory using finite uniform electron gases

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In this talk, I will start by giving a general introduction on density-functional theory (DFT) methods,[1] and describe the basic approximations made in DFT and the different families of exchange and correlation functionals used in computational chemistry softwares. Then, I will present our recent work on the construction of new types of density functionals within DFT using finite uniform electron gases.[2–6]

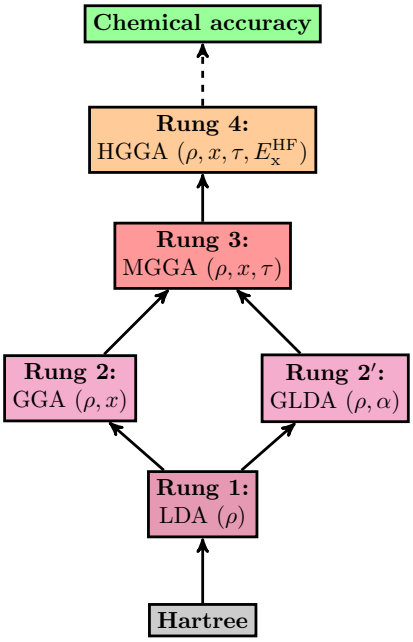


FIG. 1. Jacob's ladder of DFT revisited. $\rho$, $x$, $\tau$, $\alpha$ and $E_{\mathrm{x}}^{\mathrm{HF}}$ are the electron density, the reduced gradient, the kinetic energy density, the curvature of the Fermi hole and the Hartree-Fock (HF) exchange energy, respectively. The fourth rung corresponds to hyper GGA (HGGA) functionals.

In particular, I will show how one can construct a simple exchange functional by extending the well-know local-density approximation (LDA) to finite uniform electron gases.[7] This new generalized local-density approximation (GLDA) functional uses only two quantities: the electron density $\rho$ and the curvature of the Fermi hole $\alpha$. This alternative "rung 2" functional (see Fig. 1) can be easily coupled with generalized-gradient approximation (GGA) functionals to form a new family of "rung 3" meta-GGA (MGGA) functionals that we have named factorizable MGGAs (FMGGAs).

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