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First beyond-LSDA density functional satisfying a tight lower bound for exchange JIANWEI SUN, JOHN PERDEW, ADRIENN RUZSINSZKY, Department of Physics, Temple University — Universal constraints of density functional theory (DFT) play major roles in approximating its exchange-correlation energy ($E_{\rm XC}$). One of the prominent constraints is the Lieb-Oxford bound: $E_{xc}^{exact}[N] \geq \lambda_{xc}[N]E_x^{LDA}[N]$, where LDA stands for local density approximation, N is the electron number of systems, and $\lambda_{xc}[N]$ increases with N with an upper bound of 2.275. For ground-state 1-e systems, the above inequality reduces to $E_x^{exact}[N{=}1] \geq \lambda_{xc}[N{=}1]E_x^{LDA}[N{=}1]$ with a tight bound $\lambda_{xc}[N{=}1]$ =1.48, shedding light on the exchange energy. Our recent study (John P. Perdew's talk) shows that, to avoid violating the tight bound for any possible 1-e densities, a semilocal functional should respect it locally. We further conjecture for exchange energies that $E_x^{exact}[N] \geq \gamma_x[N]E_x^{LSDA}[N]$ with$\gamma_x[N]$ decreasing with N and $\gamma_x[N=1] = \gamma_x[N=2] = \lambda_{xc}[N{=}1]/2^{1/3}$ =1.174. Here, local spin density approximation (LSDA) is used as the reference since the exchange has a well-defined spin-scaling relation. Based on the tight Lieb-Oxford bound and the conjecture, we present a simple meta-generalized gradient approximation (MGGA) for exchange that interpolates different LSDAs for N=1 and uniform electron gas (N $\rightarrow$ infinity), respectively, and delivers excellent exchange energies for atoms. When combined with a modified PBE correlation, the MGGA yields good binding energies for molecules and lattice constants for solids.

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