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Non-empirical hyper-generalized-gradient functionals constructed from the Lieb-Oxford bound[1] MARIANA M. ODASHIMA, KLAUS CAPELLE, Universidade de Sao Paulo — A simple and completely general representation of the exact exchange-correlation functional of density-functional theory is derived from the universal Lieb-Oxford bound for Coulomb-interacting systems. This representation leads to an alternative point of view on popular hybrid functionals. A similar representation of the exact correlation functional allows to construct a family of non-empirical hyper-generalized-gradient approximations (HGGAs), departing from established paradigms of functional construction. Numerical tests and applications of these HGGAs to atoms and molecules demonstrate that even simple Lieb-Oxford based HGGAs are competitive with correlation functionals currently used in solid-state physics and quantum chemistry.

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