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A generalized gradient approximation for the Coulomb energy ALBERTO VELA, JORGE LUIS ROSAS-TRIGUEROS, Department of Chemistry, Cinvestav, SAMUEL B. TRICKEY, QTP, Depts. of Physics and Chemistry, University of Florida, JOSÉ L. GAZQUEZ, Department of Chemistry, UAM-Iztapalapa — In this contribution we generate, implement and fully test expressions for the Coulomb energy without explicit dependence of the electron density at two points in space. These approximate expressions depend solely on the density and its derivatives. The starting point is the implementation and testing of the gradient expansions suggested by Bartolotti and Parr that, to the authors' knowledge, have never been tried in molecules. One of the drawbacks of this approach is that its functional derivative diverges in finite systems. To circumvent this deficiency we will show results for a gradient expansion that incorporates several restrictions, among them to have a finite first functional derivative. Since the functionals are derived imposing some restrictions we call these functionals generalized gradient approximations to the Coulomb energy.

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