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Exchange-correlation energy functionals for electrons in two dimensions STEFANO PITTALIS, University of Missouri, E. RÄSÄNEN, University of Jyvaskila, Finaland, C. PROETTO, Freie Universitaet Berlin, Germany, M. MARQUES, CNRS, Universite Lyon I, France, E.K.U. GROSS, Max-Planck-Institut fuer Mikrostrukturphysik, Halle, Germany — Two-dimensional (2D) electronic systems have attracted vast interest since the beginning of semiconductor technology. The investigation of electronic properties of these 2D structures form a significant part of condensed matter and materials physics research. Among the available theoretical and computational methods to deal with many-electron systems is the density-functional theory (DFT). The fundamental quantity in DFT is the exchange-correlation (xc) energy functional, which embodies all the effect of the electron-electron interactions. In practice, this functional needs to be approximated. Many approximations have been developed for three-dimensional (3D) systems, where considerable advances beyond the commonly used local spin-density approximation (LSDA) were achieved. Unfortunately, most of the popular 3D approximations are inadequate for 2D systems. Hence, there is a clear need for new approximations specifically developed for 2D systems. Following this important need, efficient and practical expressions for the xc-energy of electrons in 2D are presented. Numerical results for finite systems show that the proposed functionals outperform the standard 2D LSDA.

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