

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Exchange-correlation energy functionals for electrons in two dimensions. S. PITTALIS, Free University Berlin, Germany; European Theoretical Spectroscopy Facility (ETSF); University of Missouri-Columbia, USA, E. RASANEN, University of Jyväskylä, Finland; European Theoretical Spectroscopy Facility (ETSF), C. PROETTO, Free University Berlin, Germany; European Theoretical Spectroscopy Facility (ETSF), M. MARQUES, CNRS, Université Lyon I, France; European Theoretical Spectroscopy Facility (ETSF), E.K.U. GROSS, Free University Berlin, Germany; European Theoretical Spectroscopy Facility (ETSF); Max-Planck-Institut fuer Mikrostrukturphysik, Halle, Germany — Two-dimensional (2D) electronic systems have attracted vast interest in condensed matter physics since the beginning of semiconductor technology. Density-functional theory (DFT) is among the available theoretical and computational methods to deal with many-electron systems. Fundamental quantity in DFT is the exchange-correlation (xc) energy functional. In practice, this functional needs to be approximated. Many approximations have been developed for three-dimensional (3D) systems that, unfortunately, are inadequate for 2D systems. Hence, there is a clear need for new approximations specifically designed 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 local-spin-density approximation.

Stefano Pittalis
University of Missouri-Columbia, USA

Date submitted: 22 Nov 2009

Electronic form version 1.4