Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Building improved functionals for self-consistent DFT by better treatment of electronic surface regions RICKARD ARMIENTO, KTH Physics, SE-106 91 Stockholm, Sweden, ANN E. MATTSSON, Computational Materials & Molecular Biology MS 1110, Sandia National Laboratories, Albuquerque NM 87111-1110 — We develop a specialized treatment of electronic surface regions which, via the subsystem functional approach [1], can be used in functionals for self-consistent density-functional theory (DFT). Approximations for both exchange and correlation energies are derived for an electronic surface. An interpolation index is used to combine this surface-specific functional with a functional for interior regions. When the local density approximation (LDA) is used for the interior region, the end result is a straightforward density-gradient dependent functional that shows promising results. Further improvement of the treatment of the interior region by the use of a local gradient expansion approximation is also discussed. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. [1] R. Armiento and A. E. Mattsson, Phys. Rev. B **66**, 165117 (2002).

Rickard Armiento
KTH Physics, SE-106 91 Stockholm, Sweden

Date submitted: 01 Dec 2004 Electronic form version 1.4