Abstract Submitted
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A functional designed to include surface effects into self-consistent density-functional theory calculations. A.E. MATTSSON, Comp. Materials & Molecular Biology MS 1110, Sandia National Labs, Albuquerque NM 87185-1110, R. ARMIENTO, KTH Physics, SE-106 91 Stockholm, Sweden — We present an exchange-correlation functional that enables an accurate treatment of systems with electronic surfaces. The functional is developed within the subsystem functional paradigm [1], combining the local density approximation for interior regions with a new functional designed for surface regions. It is validated for a variety of materials by calculations of: (i) properties where surface effects exist, and (ii) established bulk properties. Good and coherent results are obtained, indicating that this functional may serve well as universal first choice for solid state systems. The good performance of this first subsystem functional also suggests that yet improved functionals can be constructed by this approach. 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)

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