Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

A variational free-energy functional approach to the Schrödinger-Poisson theory FRANCISCO J. SOLIS, School of Mathematical and Natural Sciences. Arizona State University, VIKRAM JADHAO, Department of Physics and Astronomy, Johns Hopkins University, KAUSHIK MITRA, None, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University — In the numerical simulation of model electronic device systems, where electrons are typically under confinement, a key obstacle is the need to iteratively solve the coupled Schrödinger-Poisson equation in order to obtain the electronic potential. We show that it is possible to bypass this obstacle by adopting a variational approach and obtaining the solution of the SP equation by minimizing a functional. We construct the required functional and establish some of its properties. We apply this formulation to the case of narrow channel quantum wells where the local density approximation yields accurate results.

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Date submitted: 12 Nov 2014 Electronic form version 1.4