Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Density Functional Monte Carlo: an efficient way to calculate the ground state density profile of nanostructures
FONS BROSENS, KATRIJN PUTTENEERS, University of Antwerpen
— We present a method in which the Hohenberg-Kohn theorems are implemented directly by simulating the density profile using Bernouilli walkers and conserving the total number of particles during the Monte Carlo process. This leads to a much faster algorithm than, e.g., by solving the Kohn-Sham equations. The method is explained in detail and results are shown for a nanoshell which contains several millions of conduction electrons.

Fons Brosens
University of Antwerpen

Date submitted: 09 Nov 2011 Electronic form version 1.4