Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

A constraint method for variational total energy calculations of electronic excitations within the Kohn-Sham scheme[1] BABAK SADIGH, Lawrence Livermore National Laboratory — We propose a general constraint on the occupations of single-particle orbitals within (hybrid) density-functional theory that allows a variational total energy formulation for extended systems containing arbitrary electronic excitations. This method is simple to implement and is ideal for studying structural relaxations and molecular-dynamics simulations in the presence of excitations since accurate forces can be calculated via the Hellman-Feynman theorem.

[1]This work performed under the auspices of the U.S. Department of Energy by LLNL under Contract DE-AC52-07NA27344 with support from the National Nuclear Security Administration (NNSA) office of Non-proliferation Research and Development (NA-22)

Eric Schwegler
Lawrence Livermore National Laboratory

Date submitted: 29 Nov 2011 Electronic form version 1.4