

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

MP2 and RPA applied to solid state systems¹ MARTIJN MARS-
MAN, Faculty of Physics, University Vienna, ANDREAS GRUENEIS, JUDITH
HARL, GEORG KRESSE — We present *ab initio* total energy calculations at the
level of Hartree-Fock + 2nd-order Møller-Plesset perturbation theory (HF+MP2),
and the random-phase-approximation within the framework of the adiabatic-
fluctuation-dissipation-theorem (ACFDT-RPA), for extended systems under peri-
odic boundary conditions, using plane wave basis sets. We characterize and com-
pare the accuracy of these methods with respect to their description of the lattice
constants, bulk moduli, and atomizations energies of several archetypical solid state
systems. Furthermore we present calculations of HF+MP2 quasiparticle gaps and
compare them to results obtained within the GW approximation to the electronic
self-energy.

¹Supported by the Austrian Fonds zur Foerderung der wissenschaftlichen Forschung
(START grant Y218)

Martijn Marsman
Faculty of Physics, University Vienna

Date submitted: 21 Nov 2008

Electronic form version 1.4