Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

TDDFT approach with Gaussian Augmented Plane Waves
THOMAS CHASSAI, MARCELLA IANNUZZI, JUERG HUTTER, University of Zurich — The calculation of the electronic structure of large systems ($100 \div 1000$ atoms) by methods based on Density Functional Theory has recently gained a more central role. However, the extensive study of quantities like the excited states and related properties, are still out of reach, due to the high computational costs. We present the new implementation of a hybrid method, the Gaussian Augmented Plane Waves (GAPW) method, where the electronic density is partitioned in its hard and soft contributions. The former are local terms naturally expanded in a Gaussian basis, whereas the soft contributions are expanded in Plane Waves by using a low energy cutoff, without loss in accuracy, even for all electron calculations. For the calculation of the excitation energies a recently developed, time-dependent density functional response theory (TD-DFRT) technique is joined with the GAPW procedure. Given a system that is initially in the ground state, TD-DFRT derives the excitation energies from the linear response of the density to the perturbation produced by an external electrical field. We demonstrate the accuracy of the TD-DFRT-GAPW method by the comparison with other TDDFT approaches, for a set of small molecules. Our results converge very fast with the PW cutoff, which means that at the same level of accuracy we can afford much larger systems at feasible computational costs. All the implementations have been done in the framework of the CP2K program package (http://cp2k.berlios.de).

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Date submitted: 29 Nov 2004 Electronic form version 1.4