

# Combining cheap and accurate forces in *ab-initio* molecular dynamics

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We present a new technique which allows to carry on very long *ab-initio* molecular dynamics simulations. In most of the time steps, the method calculates the forces with a simplified model, the Harris functional with a minimum basis set. These forces are corrected periodically with self-consistent, converged density functional calculations. We find that it is sufficient to perform this correction relatively rarely, i. e. up to every ten steps or more, without changing significantly the static or dynamical averages, nor in fact the trajectories themselves. As the simplified model forces are hundreds of times cheaper to compute than the converged ones, those steps are virtually free, and we can extend the simulation time by a factor of ten. Although the method may be applied with any *ab-initio* scheme, it is specially well adapted to SIESTA<sup>1</sup>, because of its ability to perform a range of density functional calculations, from very fast to very accurate, using the same methodology.

<sup>1</sup> J. M. Soler et al, J. Phys: Condens. Matter **14**, 2745 (2002)