A case study in electronic structure calculations with plane waves and ultrasoft pseudopotentials: metalloporphyrins

P. Giannozzi\textsuperscript{1}, F. De Angelis\textsuperscript{2}, R. Car\textsuperscript{3}

\textsuperscript{1} NEST-INFM, Scuola Normale Superiore di Pisa, Italy
\textsuperscript{2} ISTM-CNR c/o Dip. di Chimica, Università di Perugia, Italy
\textsuperscript{3} Chemistry Dept. and PMI, Princeton University, Princeton NJ 08544, USA

We examine the practical aspects of Density-Functional electronic structure calculations for large molecules containing transition metal centers. In particular, we describe our implementation of the Car-Parrinello first-principle molecular dynamics scheme for parallel machines, using ultrasoft pseudopotentials and a plane-wave basis set. Our target systems are manganese and iron porphyrins as representatives of a large class of biologically relevant metallorganic systems. We show that our implementation of the Car-Parrinello method is powerful and well suited to parallel machines. We also show how a simple correction to the total energy allows to give a good description of charged systems in Periodic Boundary Conditions.