

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

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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.