

# **Classical and ab initio molecular dynamics for extended systems**

*Magali Benoit*

*CEMES-CNRS, 29 rue Jeanne Marvig, 31055 Toulouse Cedex, France*

*magali.benoit@cemes.fr*

## **I/ Introduction to ‘‘classical’’ molecular dynamics**

- A. Example of interaction potentials
- B. Integration of the equations of motion
- C. Boundary conditions
- D. Coulomb interaction in periodic systems : the Ewald summation

## **II/ Statistical ensembles: constant-temperature and constant-pressure MD**

- A. Nosé-Hoover thermostats
- B. Barostats

## **III/ Ab initio molecular dynamics**

- A. ‘‘Born-Oppenheimer’’ MD
- B. Plane waves vs. Localized orbitals
- C. ‘‘Car-Parrinello’’ MD
- D. Thermostats and barostats in CPMD

## **IV/ Examples of data analysis**