DIPARTIMENTO DI FISICA "E.Fermi"
UNIVERSITÀ DI PISA
CORSO DI DOTTORATO IN FISICA
VIA BUONARROTI,2 - Edificio B-C
56127 PISA - ITALY

Ciclo di lezioni per il CORSO DI DOTTORATO IN FISICA

Prof. P. Giannozzi

"Calcoli autoconsistenti in atomi, molecole, solidi."

da Martedi 20 giugno 2006 – ore 8:30-10:00
Aula F - Ed. B - Polo Didattico Fibonacci

Programma:

- **Essential Density-Functional Theory (DFT)**:
- Hohenberg-Kohn theorem, Kohn-Sham (KS) equations. Local Density Approximation (LDA): good performances, shortcomings, and reasons for both of them. The band gap problem: dependence of the energy functional upon the number of electrons, discontinuity of XC potential. Time-dependent DFT.
- **Practical DFT calculations**:
- **Atoms**: radial integration of KS equation, self-consistency - computer exercise: write (parts of) a simple code calculating the el. structure of an atom in LDA
- **Molecules**: localised basis sets Condensed-matter systems: plane waves, Supercells, Pseudopotentials, sum over the Brillouin Zone, total energy. - computer exercise: write (parts of) a simple code calculating the electronic structure of a semiconductor using empirical pseudopotentials Direct minimization of the DF Structural optimization: Hellmann-Feynman forces, Pulay forces - computer exercise: find the minimum configuration of a system described by a Lennard-Jones (LJ) interatomic potential
- **Molecular Dynamics (MD)**: Classical MD: NVE ensemble, Verlet algorithm as discretization of the Liouvillian
- - computer exercise: find MD trajectories and thermodynamical properties (p.ex. diffusion coefficient) of a LJ system; NVT and NPT ensembles, MD with first-principle interatomic potentials
- - computer exercise: phonon frequency of Si from MD in a Si supercell Car-Parrinello (CP) MD

G.Grosso