



Modelling

ENEA

ENEA-GRID High performance computational infrastructure for parallel computing, numerical analysis, visualization and data mining

Location of the infrastructure : Portici (Naples), Italy

Contact person : Silvio Migliori
Massimo Celino

Phone : +39 0636272232
+39 0630483871

E-mail : silvio.migliori@enea.it
massimo.celino@enea.it

Objectives :

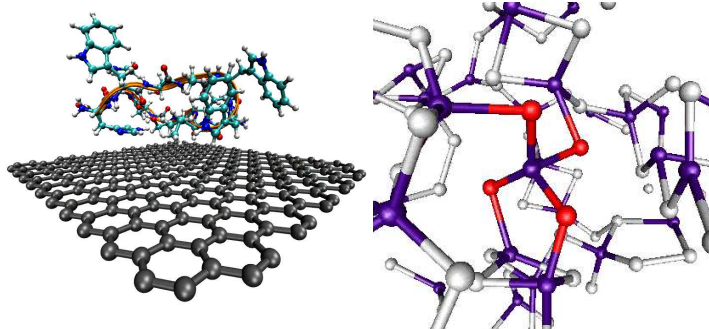
- SOPHIA virtual laboratory for PV modeling
- High performance computing and networking
- Support for the design of new materials and their characterization

Main features :

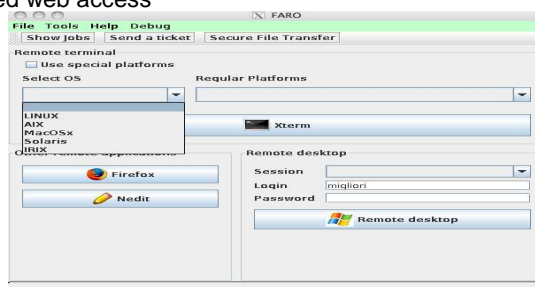
1. High performance parallel computer



2. Numerical codes for atomic scale molecular modelling of materials and complex molecules and their interaction.



3. Customized web access



4. 3D visualization and post processing analysis

5. Geographic databases / data mining

Limitations or constraints :

The availability of computing resources will be regulated by the rules adopted by ENEA in managing the access to its infrastructure and could be subject to specific negotiation.

Typical services or results :

Computer aided design of new materials and characterization of their physico-chemical properties. Several numerical codes for molecular modeling are available (Quantum Espresso, CPMD, GROMACS etc) for the atomic scale study of materials. Materials can be characterized in their crystalline, liquid and amorphous phases. Moreover the surface reactivity of nanomaterials can be addressed and their interaction with engineered peptide or polymers. Several experimental quantities can be calculated to characterize the structural and electronic properties in several thermodynamic conditions. The availability of a numerical model of the experiments is able to reduce the number of experimental tests and the overall costs of the projects.

All ENEA main computational resources are integrated in the ENEA-GRID infrastructure which provides to ENEA researchers and their partners an easy access to the available multiplatform resources. The GRID infrastructure provides a full set of services for authentication, authorization, resource discovery and management. Users can access easily to the GRID services by using an new and friendly homemade interface based on Freenx. Interconnection with other GRID infrastructures is assured by a Shared Proxy Approach for GRID Objects (SPAGO project) that offers a simple gateway to the interoperability with standard EGEE protocols. ENEA participates in EGEE initiative sharing computing resources and competences.

Examples of research projects :

- Characterization of structural and electronic properties of hydrogenated amorphous silicon
- Surface reactivity of functionalized metal oxide nanoparticles
- Adhesion properties of engineered peptide on metal crystalline surfaces.