Computational MAterials Science and Technology

CMAST Virtual Lab

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Abstract
The availability of both high performance computing platforms and efficient GRID infrastructures has opened the way to set up a Virtual Laboratory for Materials Science applications. A virtual laboratory is a friendly GRID environment where scientists and researchers from universities and industries can work together by sharing competences, software and specialized services. An example of this approach is the ENEA-GRID environment for Materials Science applications: the CMAST Virtual Lab.

Materials science applications
Materials science has received significant benefits by the availability of powerful supercomputers. These infrastructures allow the simulation of nanotechnology materials at the atomic scale with sufficient accuracy to impact on real applications. The main numerical technique used in this field is Molecular Dynamics: the equations of motion of an interacting N-particles system (ions, electrons) are iteratively solved. The evaluation of the dynamic behaviour of each particle of the system allows to evaluate its macroscopic properties and its global response to external conditions or perturbations. This is a key point because this opens the way to the computation of a large set of macroscopic quantities, often of interest for the industrial applications. Simulations can be seen as "thought experiments" which can be performed on a given system, under very well controlled conditions.

ENA CMAST Lab
CMAST is one of the ENEA Virtual Labs started as follow-up of the ENEA CRESCO Project activities. CMAST uses extensively the GRID services developed and customized by the ICT ENEA Unit (Silvio.Migliori@enea.it).

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WEB-based access to the ENEA-GRID specialized services: www.afs.enea.it/project/cmast

CRESCO tools
- Guides and tutorials for the efficient use of CRESCO platform
- How-to on ENEA-GRID

Documents
- Users can add documents to share: publications, presentations, images and movies.
- A complete and up-to-date list of the numerical packages (CPMD, Quantum Espresso, CP2K, Nwchem, GROMACS, etc.) installed in ENEA GRID is available

Photovoltaic applications: organic solar cells
Polymer solar cells are considered to be a potential candidate to solve the problem of the growing need of renewable, cost-effective energy sources. The maximum open circuit voltage for polymer solar cells is related to the difference between the HOMO of the electron donor and the LUMO of the electron acceptor. We implemented a theoretical approach to design fullerene derivatives to be used as electron acceptor in polymer solar cells. We calculated the LUMO levels of fullerene derivatives successfully used as electron acceptors and we correlated the obtained values with the Voc of the corresponding device.

Highly ionic conductive materials
The concept of short range order is largely developed to describe disordered systems, since it is based on the idea that structural correlations do not extend beyond the first shell of neighbours. However, a more extended level of structural order involving atomic nanostuctures can be found in disordered network forming systems, as those belonging to the AXn family (A= Si, Ge; X=O, S, Se). Experimentally this long range order manifests itself through the appearance of a first sharp diffraction peak in the total structure factor, properties.

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