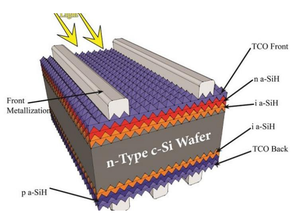
Computational Materials Science

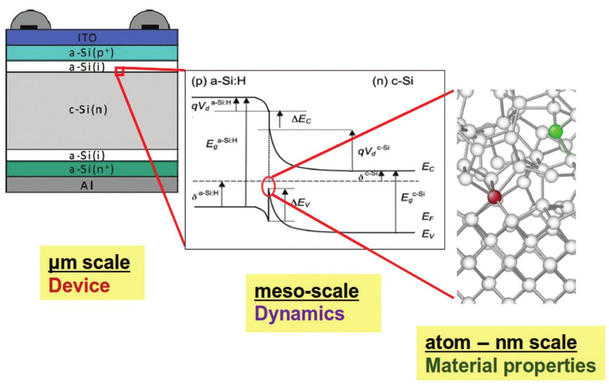
Heterogeneous Interfaces

Hetero-junction Solar Cells

Silicon hetero-junction solar cell is defined by a Crystalline Silicon wafer + semiconductor material.

Multi-scale scheme for the electronic simulation of SHJ device, to propagate atomic scale material properties at the interface to performance relevant features in the global device characteristics, via meso-scale charge carrier dynamics in the heterojunction region.





µm scale
Device

meso-scale
Dynamics

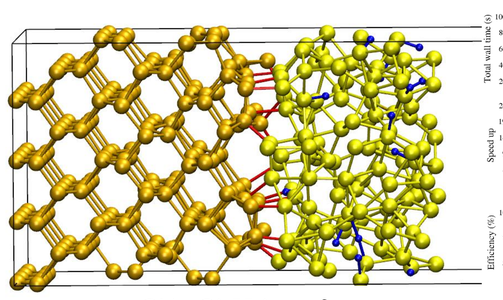
atom – nm scale
Material properties

Computational Details

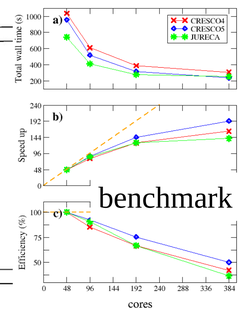
Ab-initio (DFT) Molecular dynamics

- Bulk Silicon (64 Si atoms);
- Silicon Si(001) surfaces (256 Si atoms);
- Hydrogenated amorphous Silicon a-Si:H (576 atoms): (512 Si + 64 H);
- c-Si/a-Si:H interface (336 atoms): c-Si side 192 Si, a-Si:H side 128 Si + 16 H.

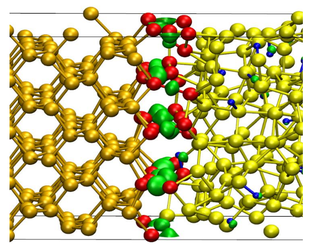
CPMD and CP2K codes on Cresco 4/5 and Juelich Jureca clusters. Typical run uses hundreds of cores (from 128 up to 1024) and GBs of disk space for I/O on parallel filesystems.

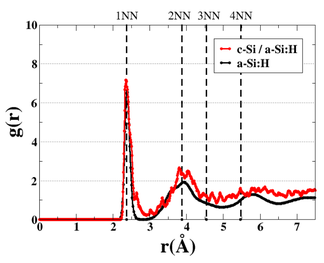


c-Si/a-Si:H interface

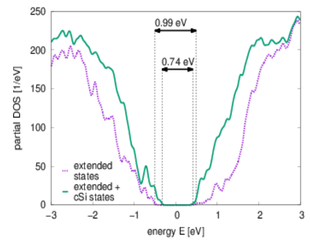


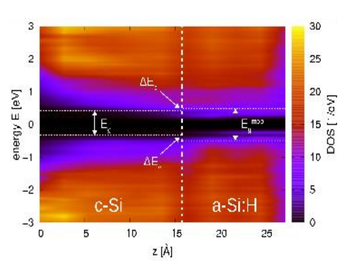
Structural Properties





Electronic Properties





- ***Ab initio description of optoelectronic properties at defective interfaces in solar cells.*** LNCS Vol. 10164 (2017) pp. 111-124.
- ***Towards a multi-scale approach to the simulation of silicon hetero-junction solar cells.*** J. Green Engineering 5 (2016) pp. 11-32.

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Molten salts as heat transfer fluids for solar applications

Molten salts (especially molten Nitrates, such as NaNO3 and KNO3) are used for heat transfer in solar energy applications (e.g. solar troughs).

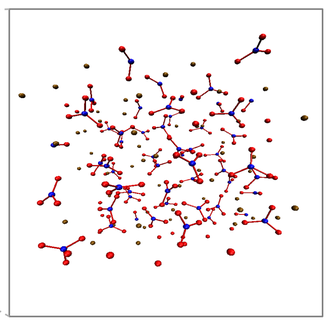
Physical and chemical properties and interaction with possible additives (nanoparticles) should be accurately investigated for the assessment of the feasibility and efficiency of a solar plant. Molecular dynamics can be a valuable tool.

Model and Computations

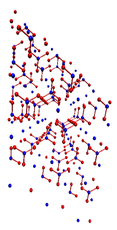
- Preliminary computations of crystal properties of NaNO3 and KNO3
- Car-Parrinello and Born-Oppenheimer MD simulations of a sample of liquid NaNO3 (270 atoms) at 500 °C

Quantum Espresso code (PW+psp DFT) used on Cresco4. Typical run: 256 cores, 0.25 ps/day of MD.

Liquid

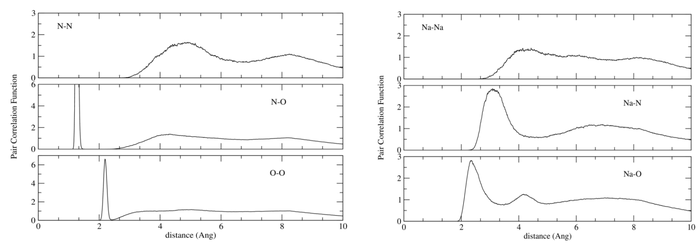


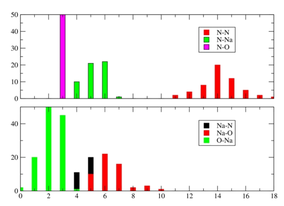
Solid



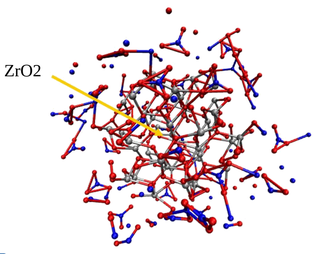
Results

- Density: 1.745 g/cm^3
- Computation of pair distribution functions, coordination number, self-diffusivity
- No dissociation NO3 → NO2 in the sample of pure salt
- Possible surface reactions in salt added with ZrO2 nanoparticles





Coordination number



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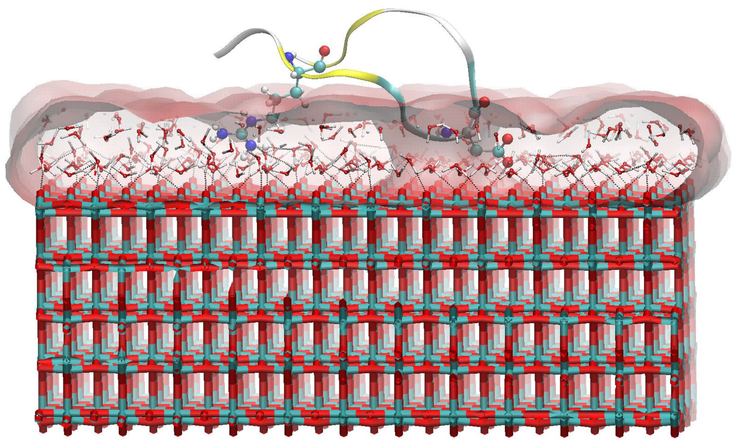
Dynamics of Peptide-TiO_2 Interfaces

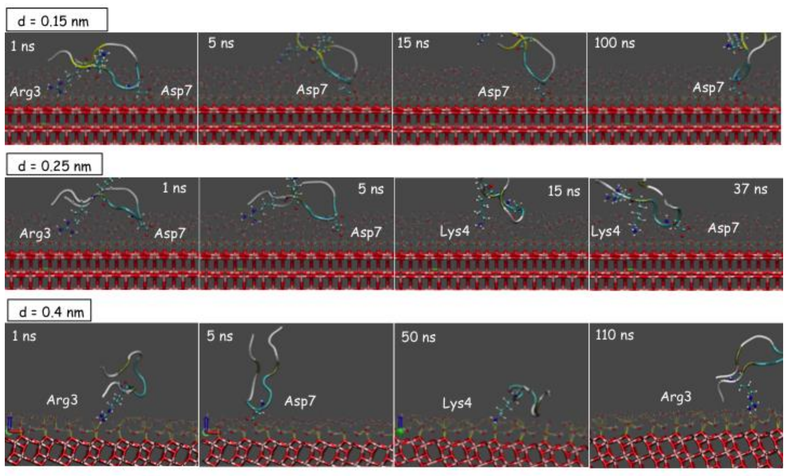
Understanding the molecular level mechanisms occurring at bioinorganic interfaces is of critical importance for the development and design of new bio-derived material.



Here we report part of the results published by Polimeni et al. [1]. The results were obtained by using molecular dynamics (MD) simulations in order to investigate the dynamics at the interface between a specific peptide sequence (RKLPDA) and a TiO2 anatase surface.

Simulations on CRESCO

Some of these simulations were performed on the CRESCO platform with the GROMACS 4.5.5 package, using the OPLS-AA force field implemented with the Lennard-Jones and Coulomb parameters for Ti and O atoms.



Results

The diffusion of the peptide and the minimum distances from the TiO_2 surface to the whole peptide as a function of simulation time for the three different MD simulations was monitored. In the simulations, the adsorption mechanism is characterized by diffusion of the peptide from the bulk water phase towards the TiO_2 surface. The peptide anchors to the surface by the recognition of water layers at the interface *via* the charged groups of its side-chains. During the simulations the peptide samples a number of anchored and dissociated states, in agreement with the experimentally observed weak bound of the synthetic minTBP-1 peptide to Ti (K_d=13.2 mM).

[1] Polimeni M., Petridis L., Smith J.C, Arcangeli C. 2017. Dynamics at a Peptide-TiO2 Anatase (101) Interface. J. Phys. Chem. B. 121(38):8869-8877

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