High performance computing to design new materials for energy applications: the c-Si/a-Si:H interface for PV technology

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ENEA ICT and HPC infrastructures

Casaccia Research Centre

The headquarter in Rome

Portici computing centre

ENEA ICT and HPC infrastructures

ENEA
AGENZIA NAZIONALE PER LE NUOVE TECNOLOGIE, L'ENERGIA E LO SVILUPPO ECONOMICO SOSTENIBILE

Remote use of instruments

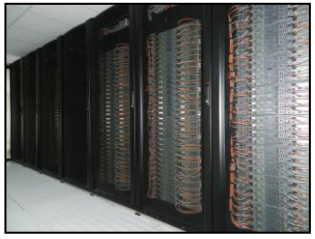
Storage

E-learning

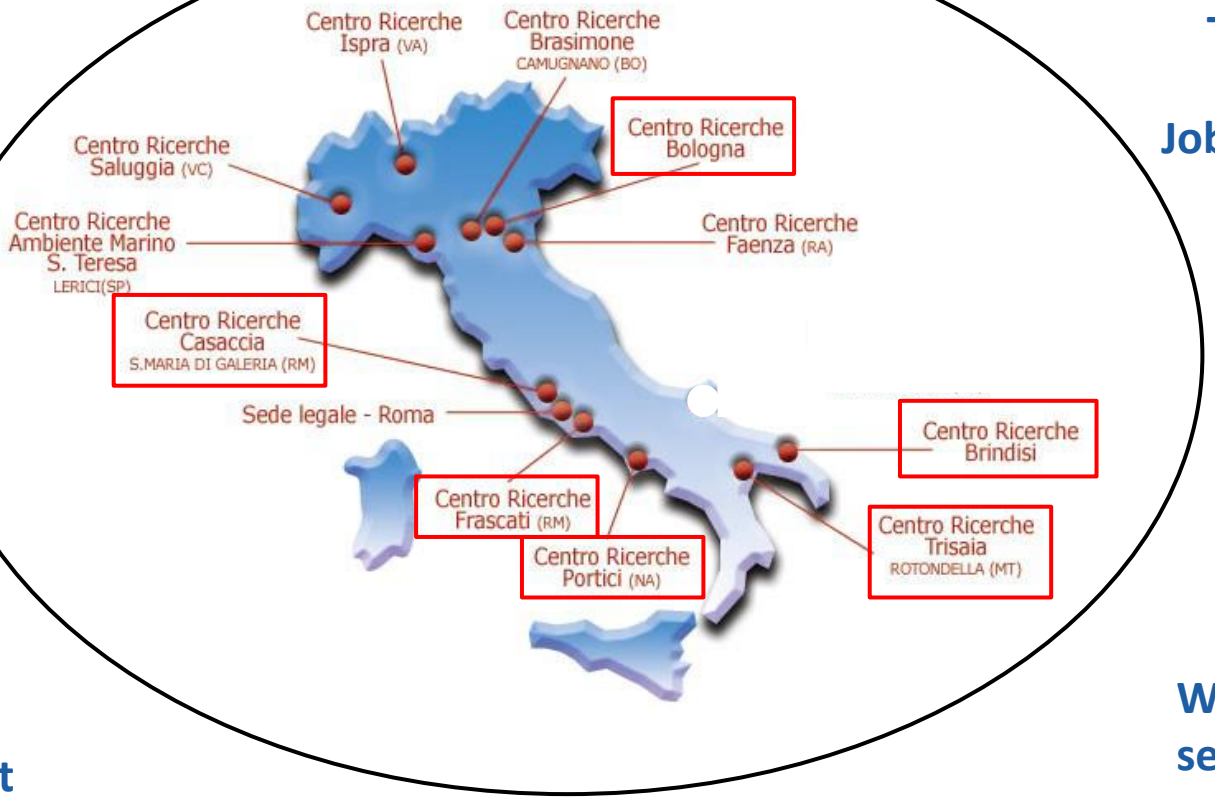
Databases

Ticketing

Supercomputers



Job monitor



Virtual Labs

User support

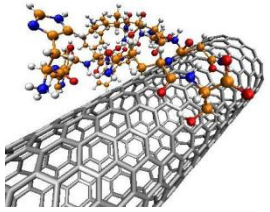
Software management

Installation
Update
Management

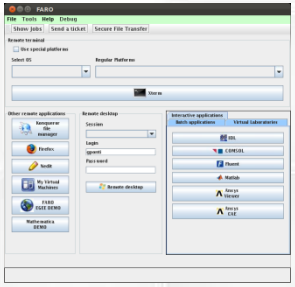
Collaborative tools

Doc sharing, Web conferencing

Visualization tools



Web access to HPC services



ENEA ICT and HPC infrastructures





www.cresco.enea.it

CRESCO3 (*20 Tflops, 2016 cores)*
- *84 nodes 2x12 cores AMD 6234 @2.4 GHz;*

CRESCO4 (*100 Tflops, 4864 cores)*
- *304 nodes 2x8 cores Intel E5-2670 @2.6 GHz;*

CRESCO5 (*25 Tflops, 640 cores)*
- *40 nodes 2x8 cores Intel E5-2630v3 @2.4 GHz;*

***Nodes** with 64 GB RAM, 500GB SATA II disk, IB QDR 40 GB/s,* 2 GE interfaces.

CRESCO4 Special Section (*17 Tflops)*
- *5 nodes 2x6 cores Intel E5-2643v2 @3.5 GHz, 768 GB RAM, 1TB SATA II disk, IB QDR 40 GB/s,* GE interfaces.
- *4 nodes 2x10 cores Intel E5-2680v2 @2.8 GHz, 64 GB RAM, 500GB SATA II disk, IB QDR 40 GB/s,* 2 GE interfaces.

5 PHI 5110P (60 cores,1Tflops) boards
3 Nnvidia K40M (1.43 Tflops) boards

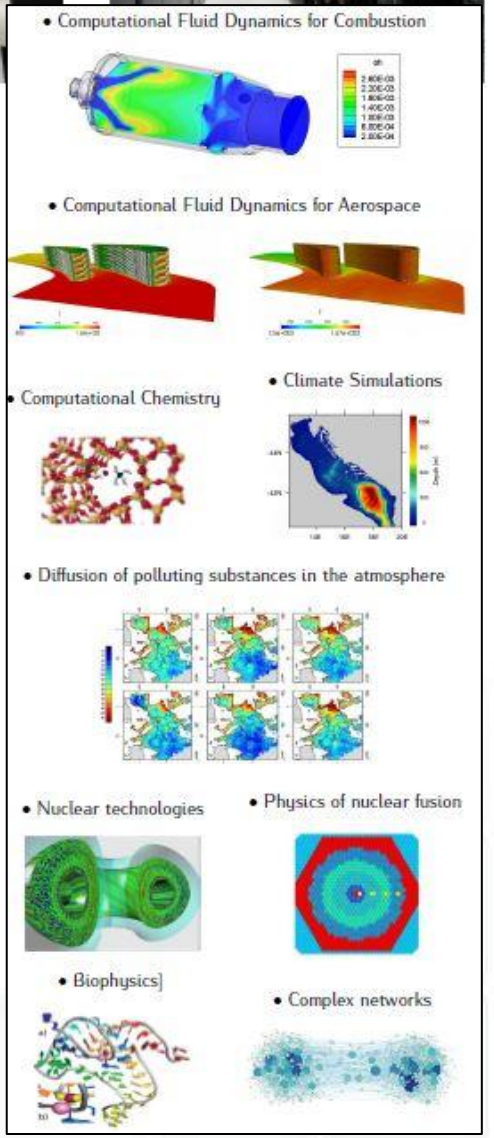
CRESCOF, CRESCOC, CRESCOB (760 cores)

➢ **2017 a new HPC cluster ~0.5PFlops in the framework of ENEA/CINECA agreement on Tier0/Tier1 roles in the Italian national HPC environment.**

- ✓ More than 350 users from academy, industries and research centres
- ✓ Several thematic Virtual Labs

CRESCO infrastructure for:

- ✓ **EoCoE:** European Energy oriented Centre of Excellence for computing applications
- ✓ **EXTREME:** European network for the substition of critical raw materials working in extreme conditions
- ✓ **EUROfusion:** European organization for the fusion development
- ✓ **EDOC:** Italian education on cloud project
- ✓ **COBRA:** Italian cultural heritage
- ✓ **DC4Cities:** European energy adaptive data centres



ENEA ICT and HPC infrastructures

ENEA–CINECA agreement for EUROfusion

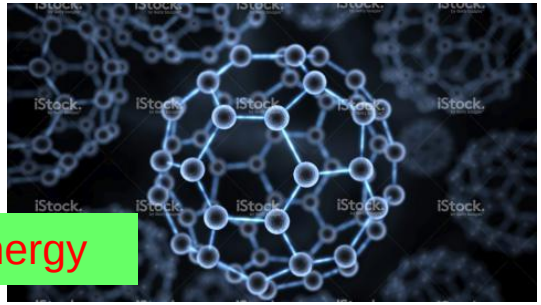
- ENEA–CINECA won the European call launched by EUROfusion, the European Consortium for the Development of Fusion Energy, for the procurement of a several PFlops HPC system;
- On July 1st, 2016 the new machine MARCONI–Fusion, exclusively devoted to studies of interest for nuclear Fusion topics, started its operations;
- MARCONI-Fusion is a 1Pflops partition of MARCONI, CINECA's 2Pflops peak facility;
  - ✓ Lenovo NeXtScale, Intel OmniPath Cluster, 1.512 nodes, 54.432 cores, 2 x 18-cores Intel Xeon E5-2697 v4 (Broadwell) @ 2.30 GHz;
- An upgrade of the machine is foreseen for next year, when the total computational power will be pushed to about 5 Pflops;

ENEA offer support to users in the design and benchmark of applications to be ported on Marconi-Fusion

European Centre of Excellence EoCoE

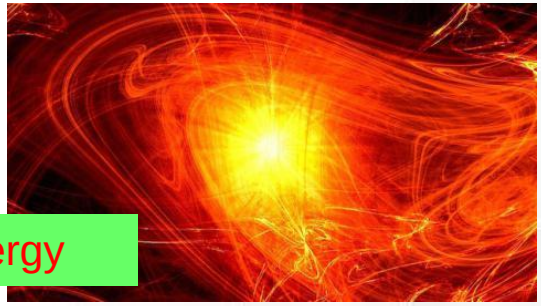
- EoCoE
  - Horizon2020 Energy oriented Centre of Excellence for computing applications, www.eocoe.eu
  - EoCoE uses the impressive potential offered by the ever-growing HPC computing infrastructure to foster and accelerate the European transition to a reliable low carbon energy supply.
  - Four pillars (Meteorology, Materials, Water and Fusion) are targeted to enhance their numerical modelling capabilities by a transversal multidisciplinary effort providing both high-end expertise in applied mathematics and access to high-end HPC infrastructures.

Meteorology for energy



Materials for energy

Water for energy



Fusion for energy

CMAST, Computational MAterials Science and Technology Virtual Lab

A CRESCO Virtual lab

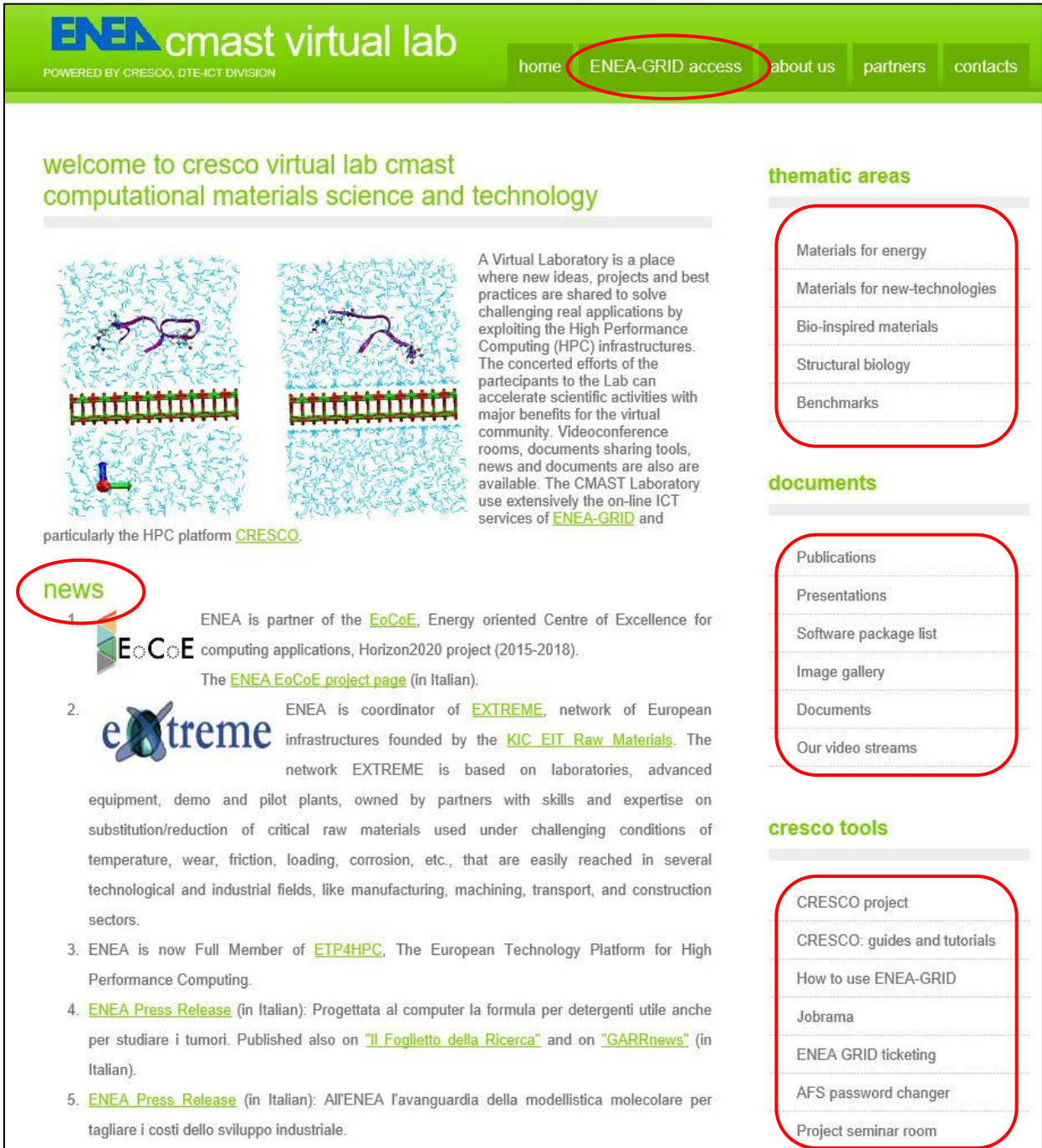
CMAST Virtual lab is composed by all the CRESCO users involved in computational projects in the field of:

- materials science
- nanotechnology
- structural biology

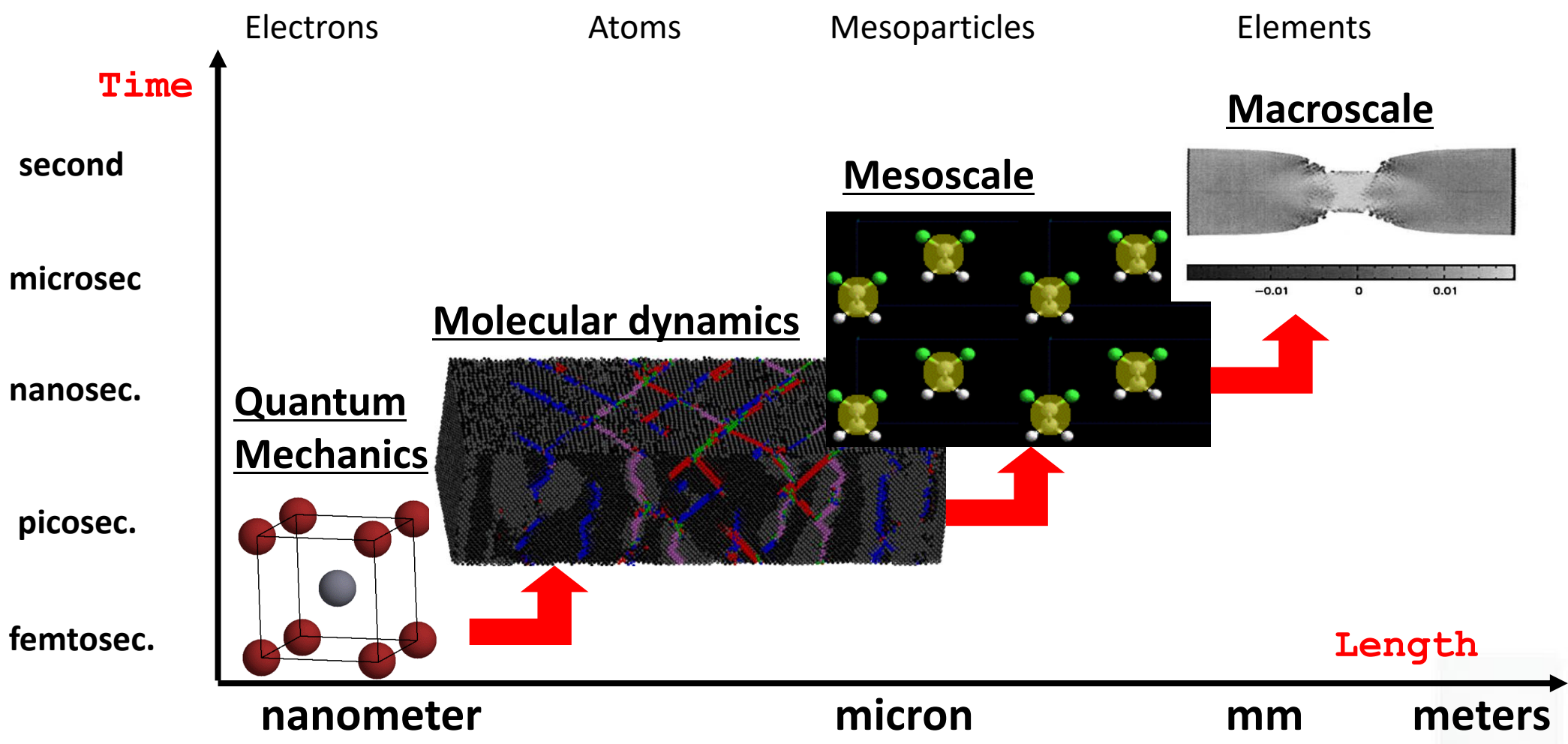
CMAST provides:

- friendly access to CRESCO
- numerical codes
- numerical libraries
- documents
- papers
- guides and education
- collaborative frameworks
- expertises

www.afs.enea.it/project/cmast



Multiscale modeling of materials



GOALS

- To understand the molecular level origin of macroscopic properties
- To predict the behaviour of materials
- To design new materials or devices with improved performance

Molecular dynamics simulations

MODEL

System Hamiltonian
Interaction between particles
Bonded and non bonded interactions
Forces on particles

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i<j}^{N} u(r_{ij}) + \ldots + U_{ext}$$

$$\mathbf{F_i} = -\sum_{j=1, j\neq i}^{N} \frac{\partial u_{ij}(r)}{\partial \mathbf{r}_{ij}}$$

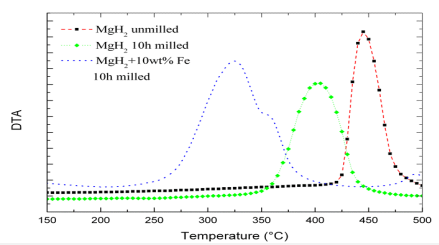
INTEGRATOR

Propragation through phase space
Finite difference schemes
Equation integrators
Numerical stability

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \quad , \quad \dot{q}_i = \frac{\partial H}{\partial p_i}$$

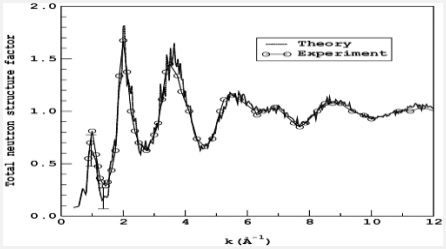
STATISTICAL ENSEMBLE

Thermodynamical conditions
Microcanonical ensemble
Canonical ensemble
Isothermal-isobaric ensemble



RESULTS

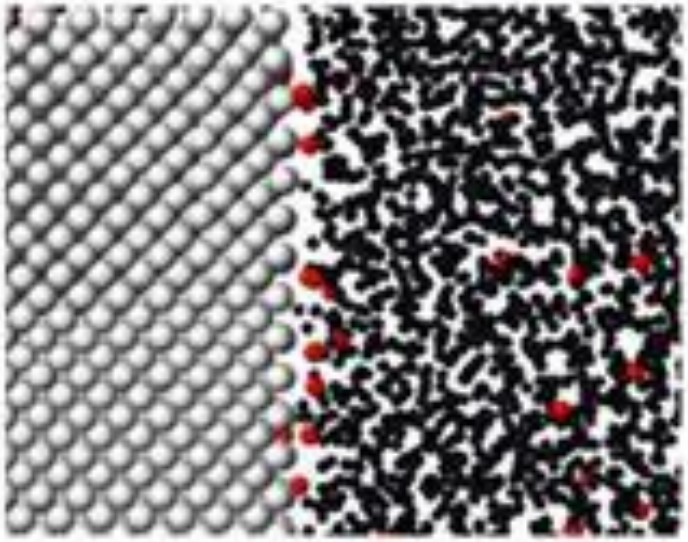
Thermodynamics and statistical mechanics
Internal energy, pressure, temperature
Response functions, correlation functions, linear response theory



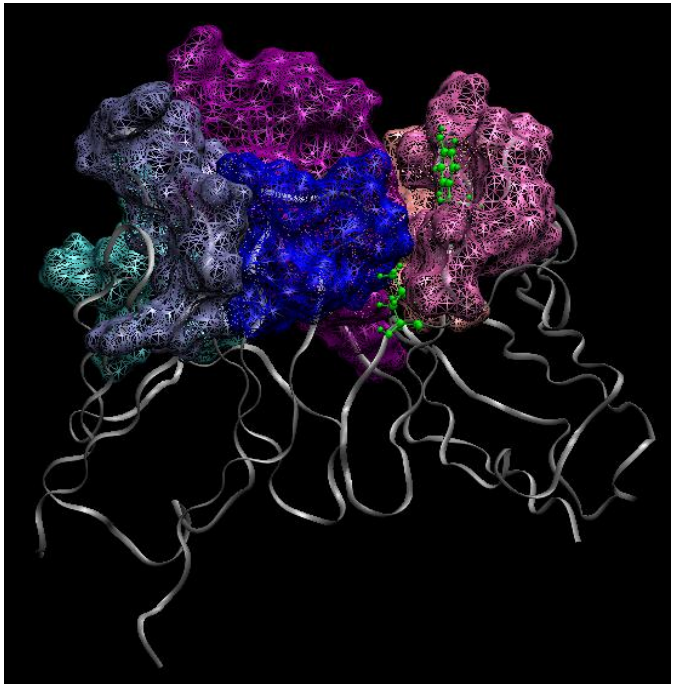
Molecular modeling of materials

ENEA molecular modeling activities in the field of

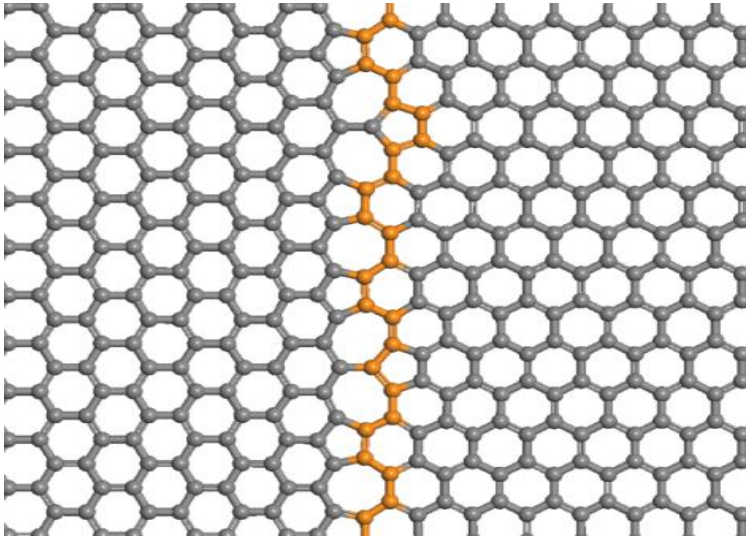
Materials



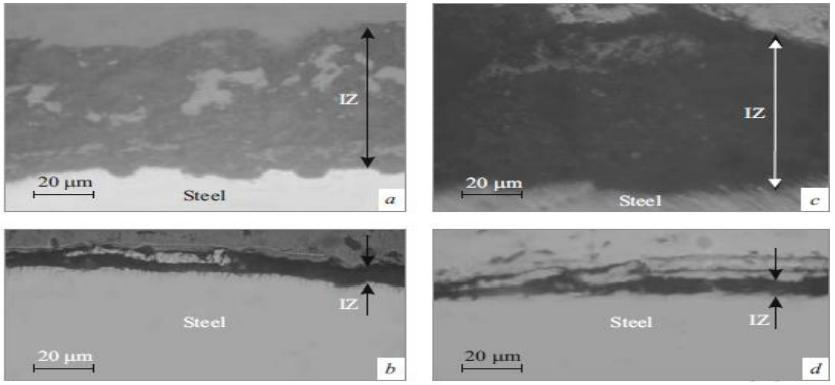
Biomolecules



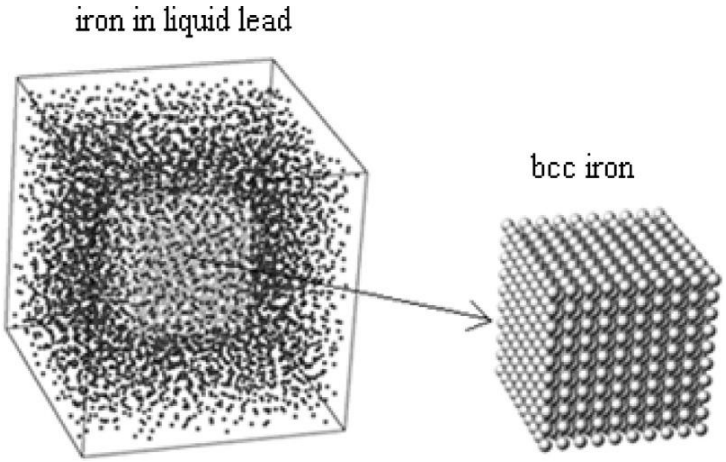
Nanotechnologies



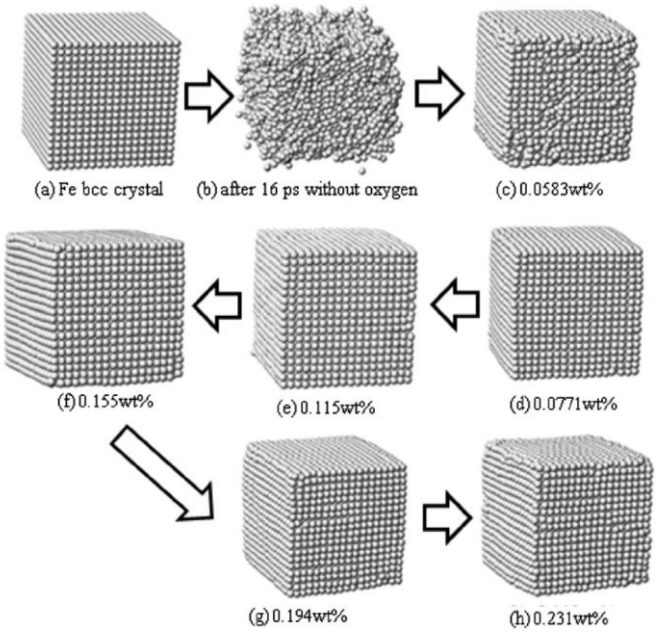
Corrosion: liquid Pb on Fe

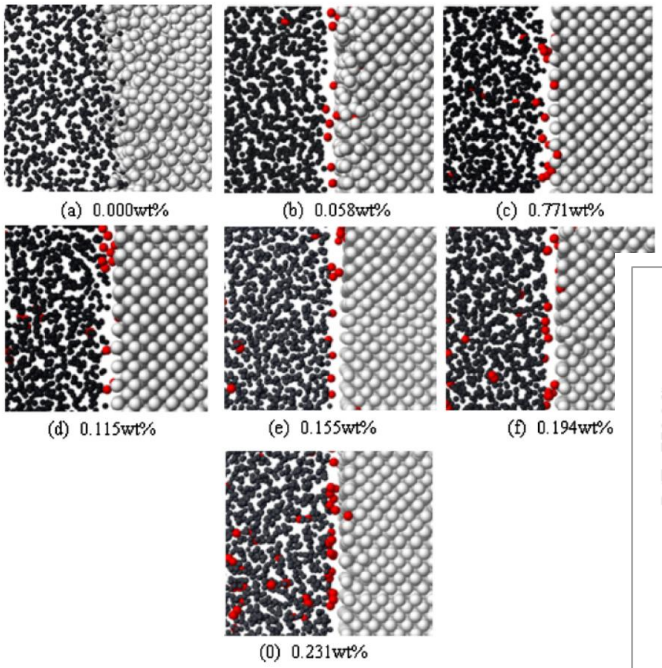


From experiment to the model

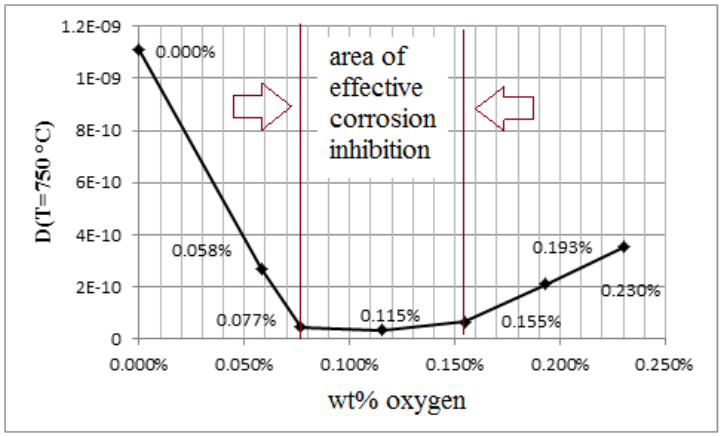


Effect of the oxygen in the liquid Pb



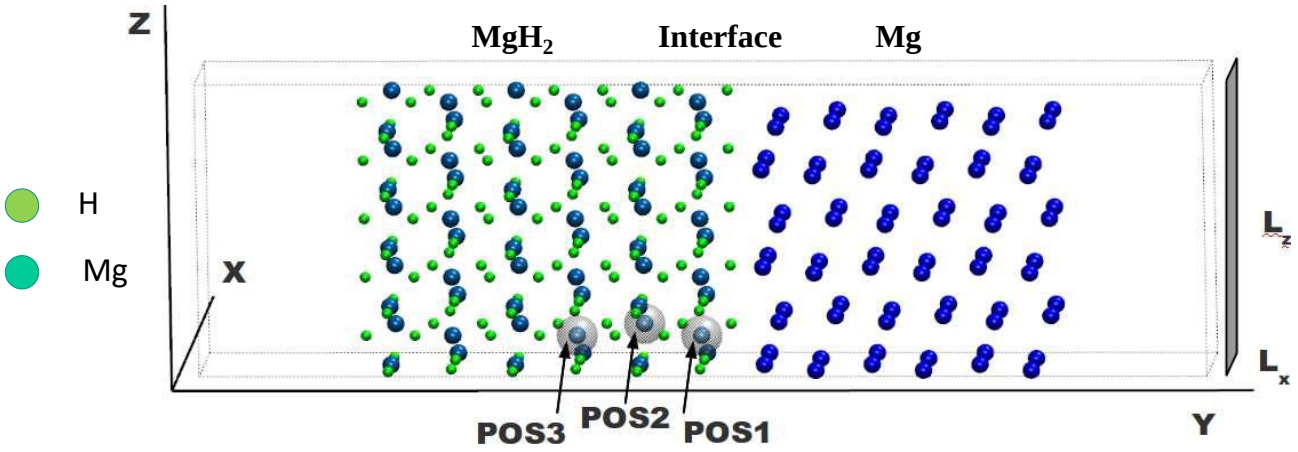


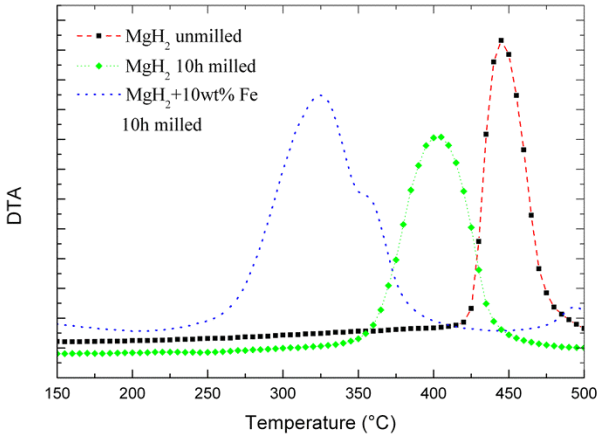
50000 atoms
Codice Moldy



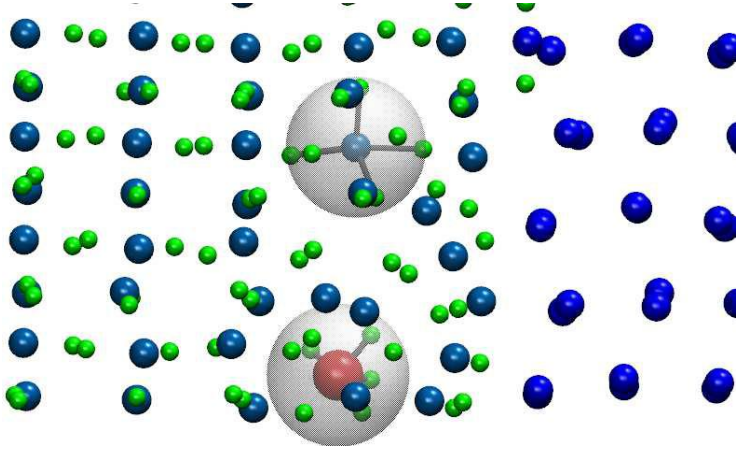
*"***Inhibition of iron corrosion in high temperature stagnant liquid lead: A molecular dynamics study** *",*
A.Arkundato, Z.Suud, M.Abdullah, W.Sutrisno, M.Celino,
Annals of Nuclear Materials 62 (2013) 298.

Hydrogen desorption from MgH_2 : the role catalysts





Ab-initio molecular dynamics of MgH2 system with the catalyst

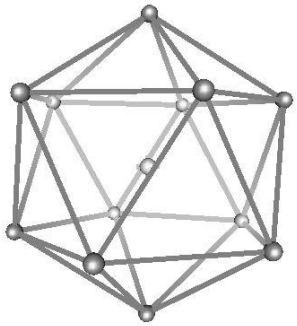


Deformation and destabilization of the catalyst leading to hydrogen displacement toward the interface.

Catalyst	POS1 W	POS1 ΔW	POS1 ΔH	POS2 W	POS2 ΔW	POS2 ΔH	POS3 W	POS3 ΔW	POS3 ΔH
Fe	776	171	4.42	614	9	4.46	606	1	4.40
Co	863	258	5.16	637	32	4.79	615	10	4.62
Ni	928	323	3.35	694	89	2.46	654	49	2.18
Nb	911	306	7.10	679	74	6.41	647	42	6.26
Pd	966	361	2.32	685	80	1.02	635	30	0.70

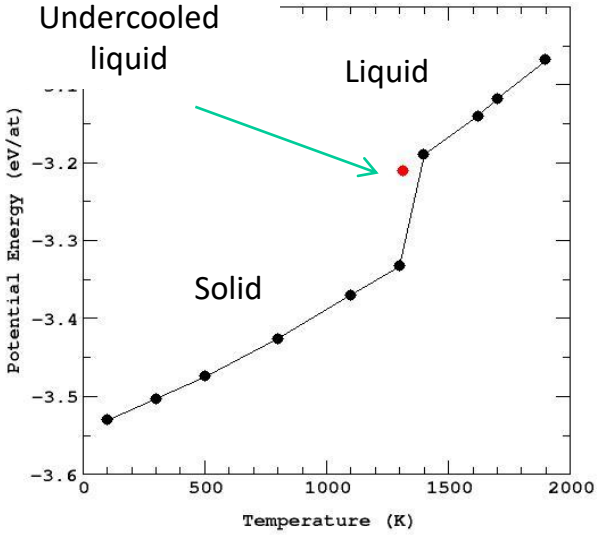
W (mJ/m2): work of adhesion of the systems with catalyst in positions POSx.
ΔW (mJ/m2): variation of W compared to the interface without catalyst.
ΔH (eV) : the formation energy of the substitutional defect.

Liquid and undercooled simple metals



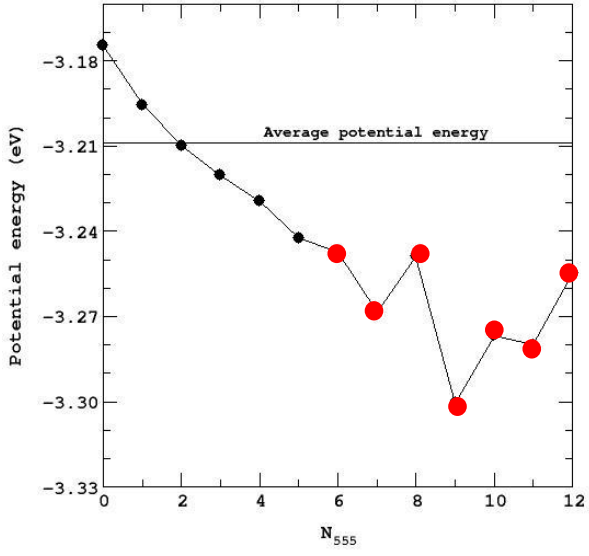
The stability of undercooled simple metals is still an intriguing problem for materials science and technology. There is not consensus on the role played by the **icosahedral short range order during undercooling**. The scenario is even less clear for **undercooled metals under external pressure**. Extensive molecular dynamics simulations, based on an empirical tight-binding interatomic potential, are performed to explain experimental results recently obtained on liquid and undercooled liquid copper and nichel.

Solid-liquid phase transition changing temperature and production of the undercooled liquid metal

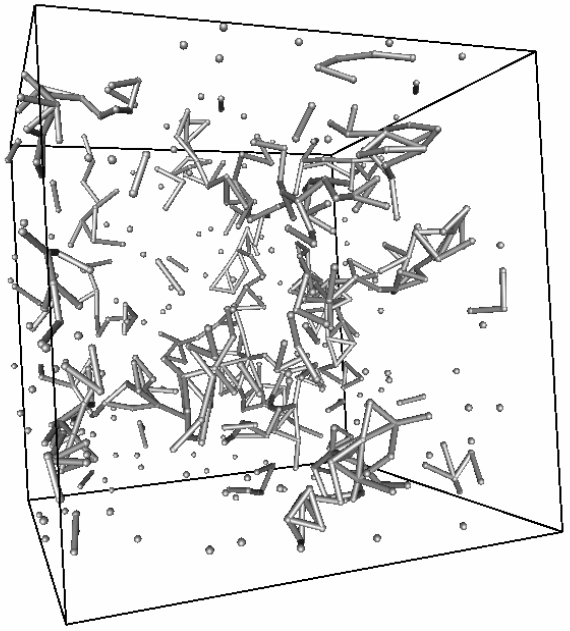


Copper

Contribution (in red) of icosahedral clusters to the stability of the liquid phase:
icosahedral order provides the largest contribution to overall stability of the liquid metal



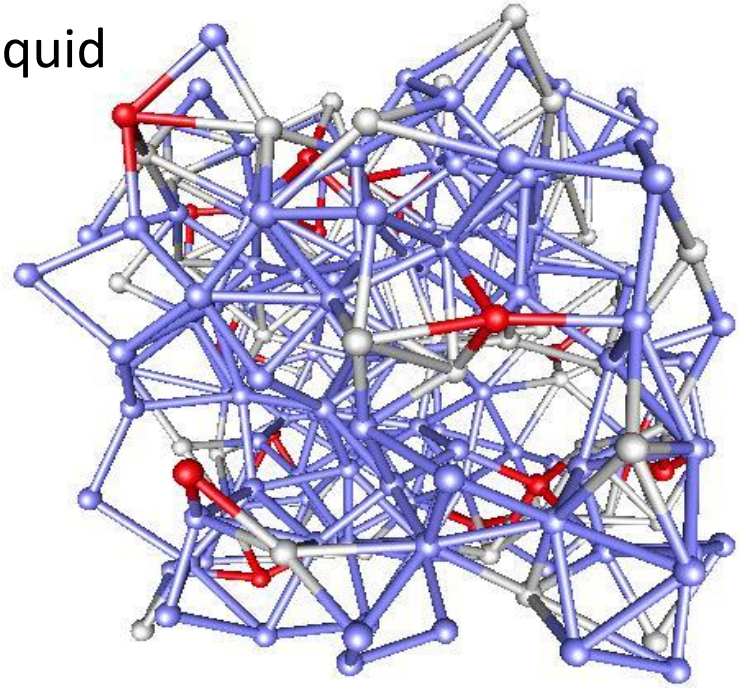
Toward increasing icosahedral order

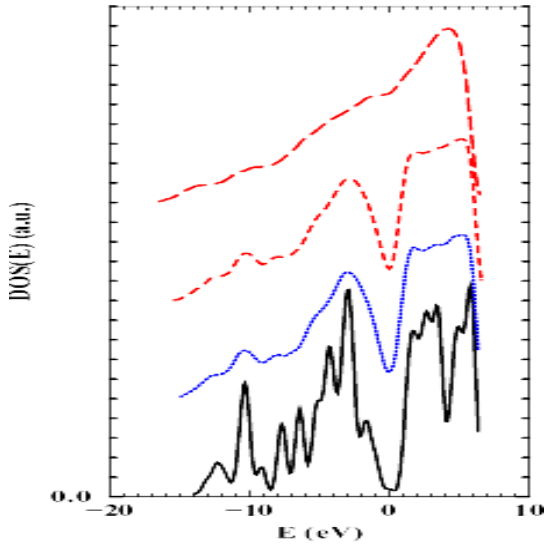


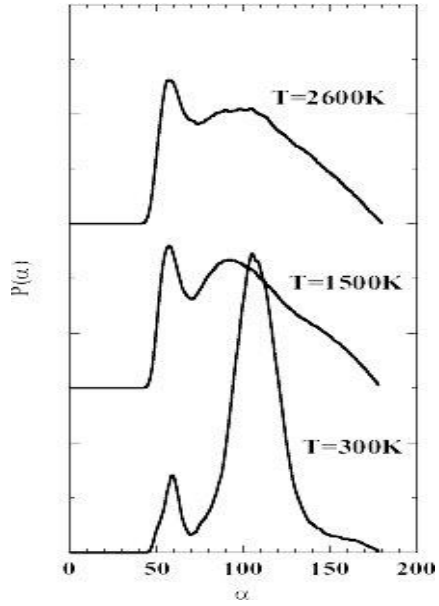
Distribution of icosahedra cluster inside the liquid copper

Amorphous silicon

Liquid



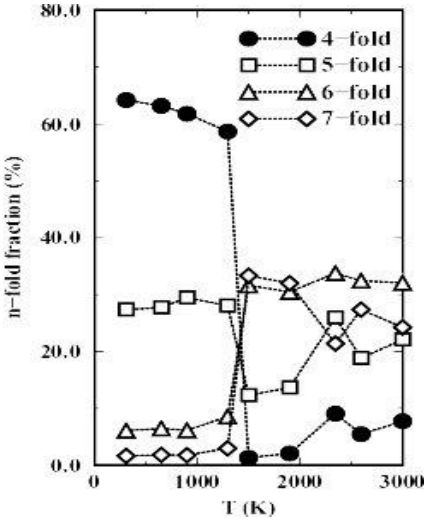


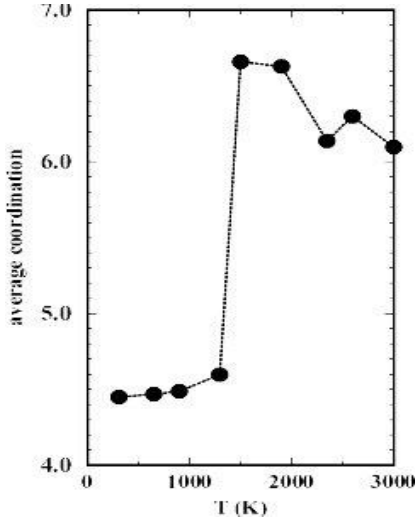


4-fold coordination

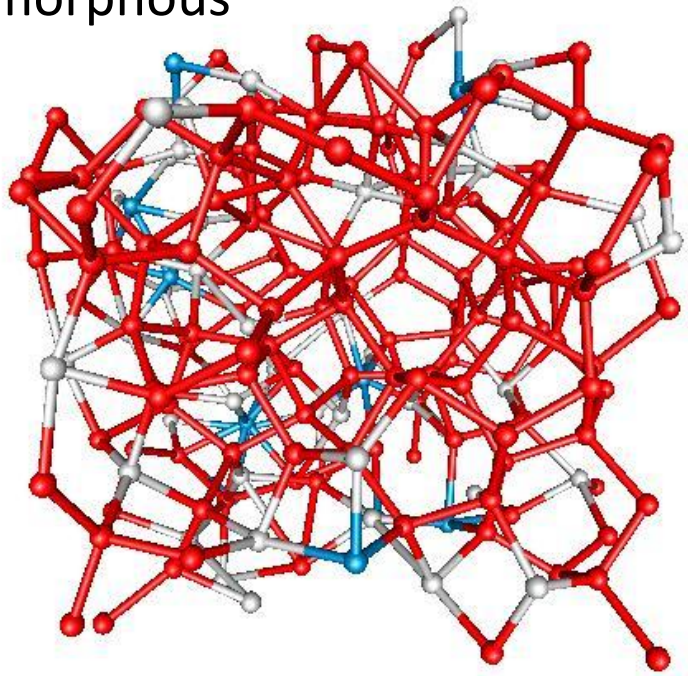
5 -fold coordination

6-7-fold coordination





Amorphous



Hetero-junction solar cells

Towards a Multi-scale Approach to the Simulation of Silicon Hetero-junction Solar Cells

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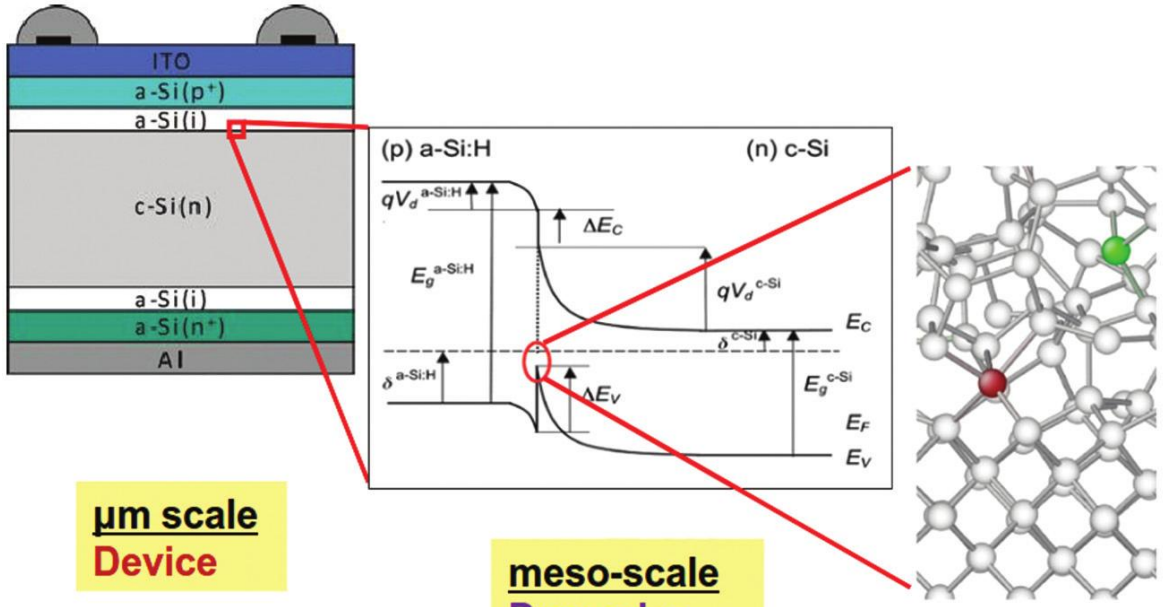
Received 5 November 2015; Accepted 3 June 2016;
Publication 1 August 2016

Journal of Green Engineering, Vol. 5, 11–32.
doi: 10.13052/jge1904-4720.5342

Hetero-junction solar cells

❑ Silicon hetero-junction solar cell

- ➢ crystalline Silicon wafer + semiconductor material
- ➢ opto-electronic simulations
  - ✓ Optical part
  - ✓ Electronic part



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

µm scale
Device

meso-scale
Dynamics

atom – nm scale
Material properties

The atomic and electronic structure at the amorphous crystalline interface is the starting point of any investigation targeting the impact of the interface properties on the device characteristics.

Hetero-junction solar cells

Computational details

- PWscf code of Quantum Espresso Suite;

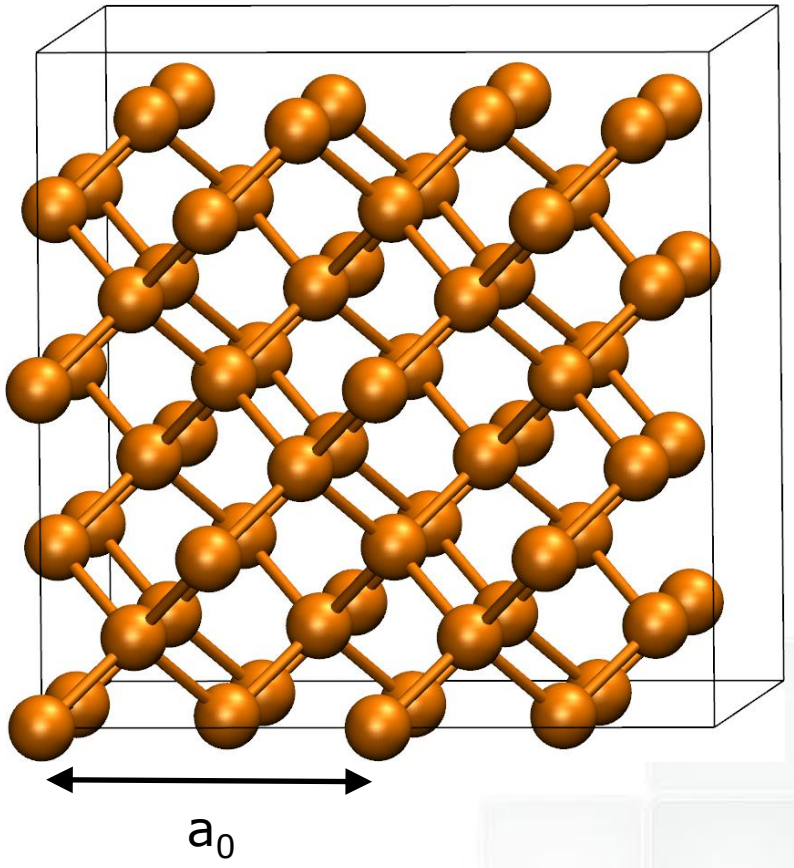
  PWscf performs many different kinds of self-consistent calculations of electronic structure properties within Density-Functional Theory (DFT), using a Plane-Wave (PW) basis set and Pseudo-Potentials (PP).

- Pseudopotentials;
  - ✓ Si.pbe-n-rrkjus_psl.0.1.UPF;
  - ✓ H.pbe-rrkjus_psl.0.1.UPF;
  - ✓ Ultrasoft PP type;
  - ✓ Method: Rappe Rabe Kaxiras Joannopoulos;
  - ✓ Perdew-Burke-Ernzerhof (PBE) exch-corr. functional type.
- Ecut wfc = 40.0 Ry;
- Ecut rho = 240.0 Ry;
- Periodic Boundary Condition (PBC);
- Born-Oppenheimer molecular dynamics (BOMD) simulations;
- NVT simulations.

Bulk silicon

- 2x2x2 array of fcc conventional cells
- 64 atoms supercell
- 4x4x4 Monkhorst-Pack uniform K-points grid

		Calculated	Exp.
a_0	(Å)	5.47	5.43
B	(Gpa)	89	99
C_{11}	(Gpa)	153	168
C_{12}	(Gpa)	57	65
C_{44}	(Gpa)	75	80

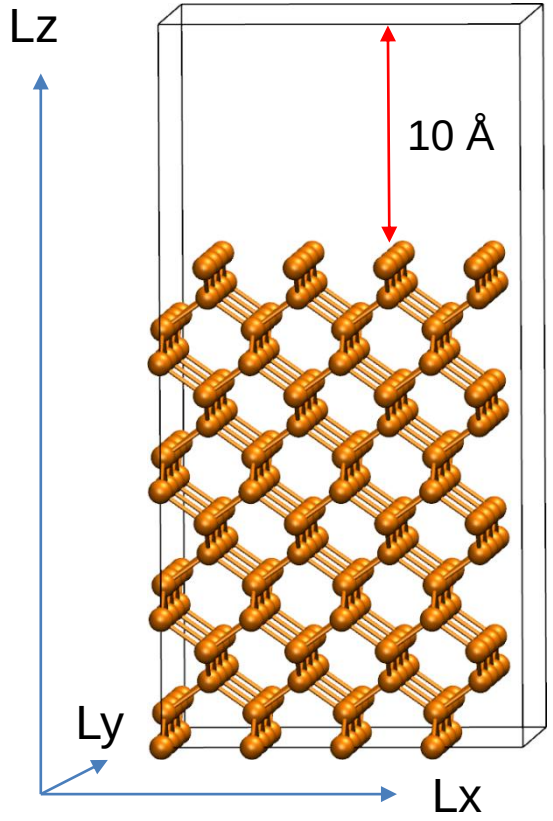


Silicon Si(001) surfaces: c-Si

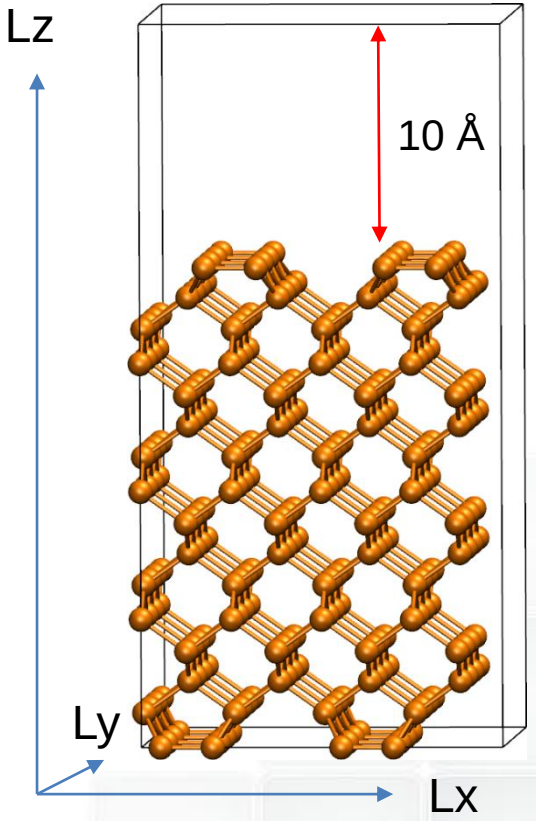
- 32 fcc cells
- 256 atoms supercell
- (001) surface in z direction
- Lx = Ly =15.46 Å, Lz =2*Lx
- 2x2x1 Monkhorst-Pack uniform K-points grid

		Unrec. p(1x1) Ideal	Recon. p(2x1) Sym.
Surf. ener.	J/m^2	2.12	1.42
Refs.		2.39	1.45
Ener. Diff.	eV/ dimer		1.5
Refs.			1.5-2.1

Unreconstructed p(1x1) ideal



reconstructed p(2x1) sym.

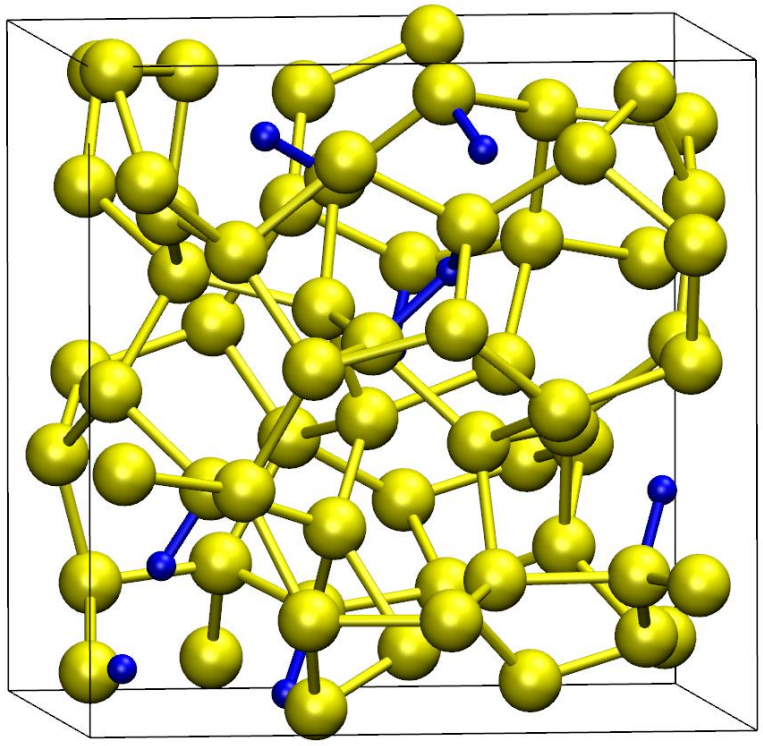


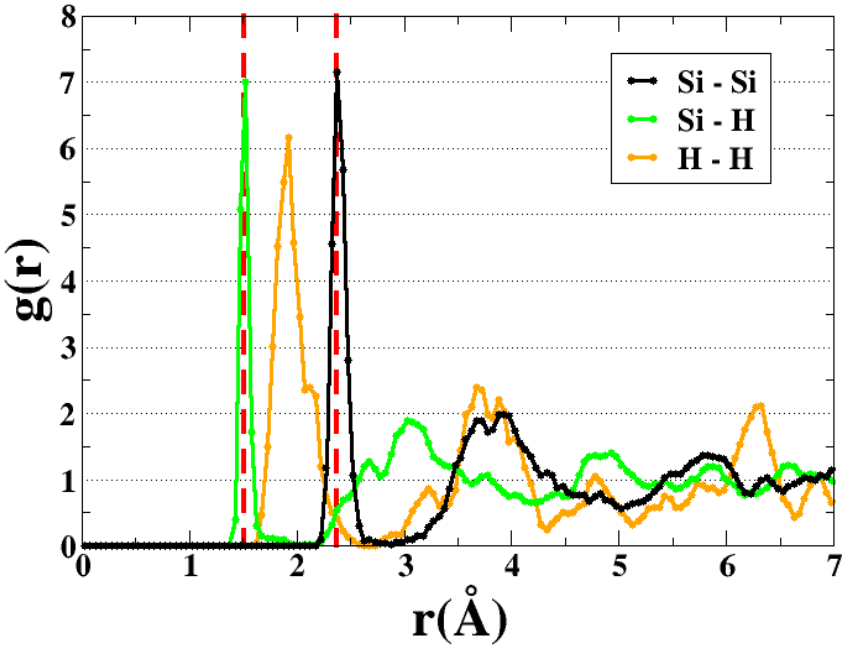
Hydrogenated a-Si

- Cubic cell L= 11.06 Å
- 72 atoms (64 Si + 8 H)
- 2.214 g/cm^3
- BOMD at 300 K
- t = 6.5 ps

Peaks at
1.51 Å (Si-H)
and
2.37 Å (Si-Si)

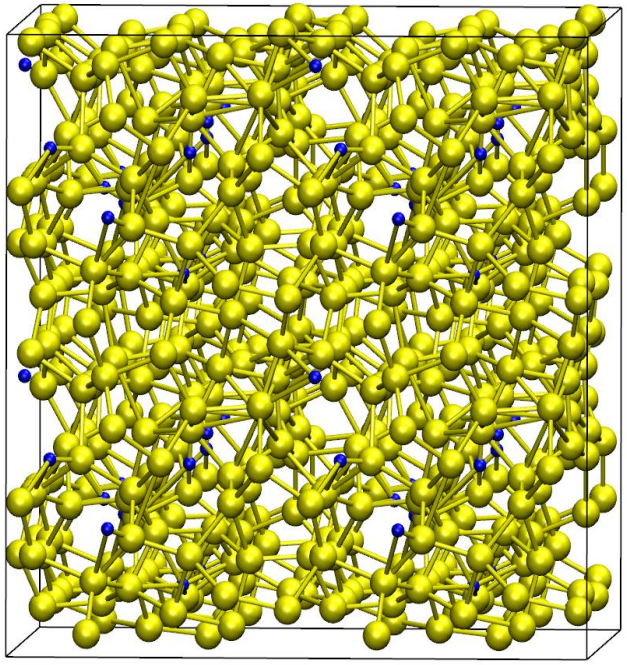
Coor.	n (%)	Env.	
1	0	Si1H0	0
2	0	Si2H0 Si1H1	0 0
3	4 (6,3)	Si3H0 Si2H1	4 0
4	58 (90,6)	Si4H0 Si3H1 Si2H2	57 1 0
5	2 (2,1)	Si5H0 Si4H1 Si5H2	1 1 0

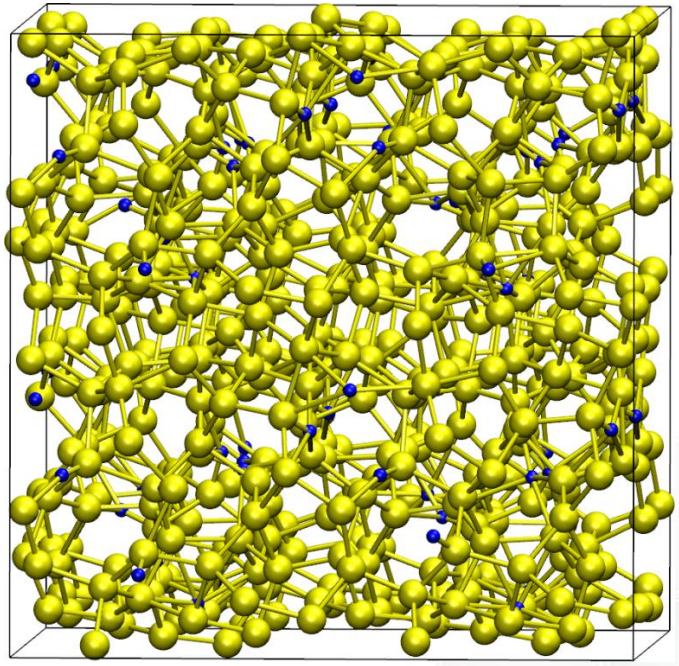




Hydrogenated a-Si

- A 8x replica of the previous system
- Cubic cell L = 22.12 Å
- 576 atoms (512 Si + 64 H)
- 2,214 g/cm^3
- Annealing 300 K => 600 K => 300 K
- t = 60 ps (CP2K code)





Starting configuration

Relaxed configuration

Hydrogenated a-Si

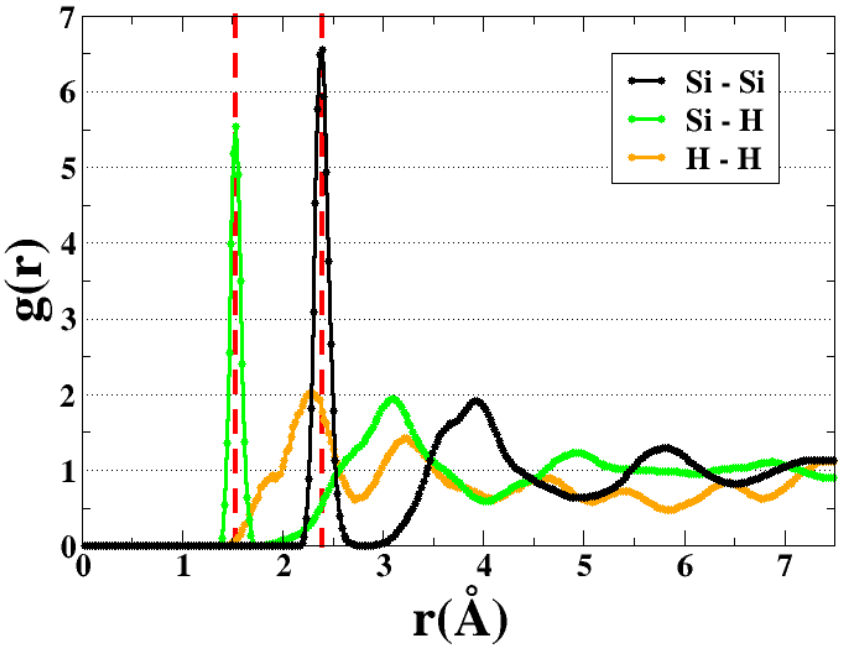
❑ CP2K Computational details

- ➢ Quickstep code of CP2K

  CP2K is a quantum chemistry and solid state physics software package that can perform atomistic simulations with different modelling methods such as DFT using a mixed Gaussian and plane wave approach.

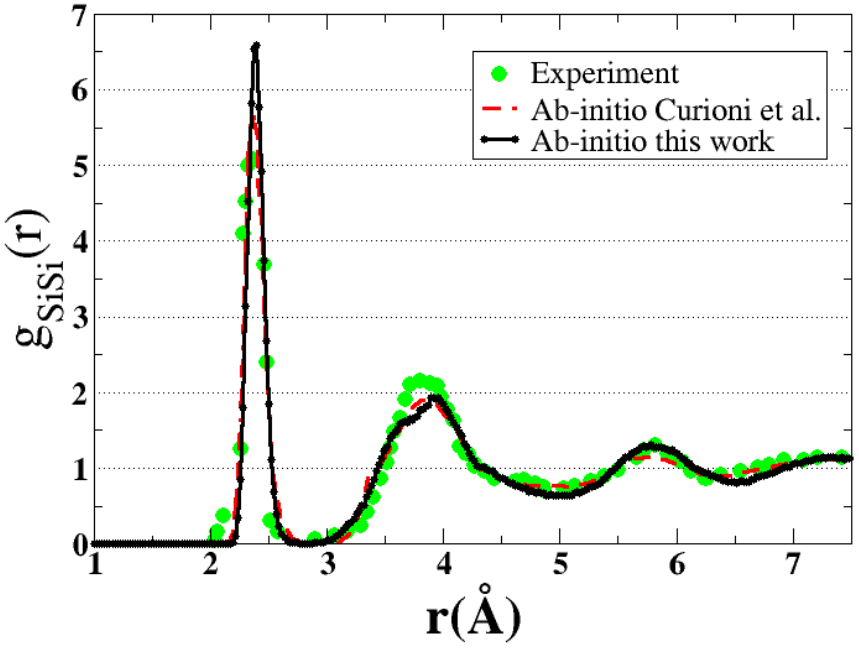
- ➢ Pseudopotentials;
  - ✓ Goedecker-Tetter-Hutter type;
  - ✓ Perdew-Burke-Ernzerhof (PBE) exch-corr. functional type.
- ➢ Gaussian Basis: optimized TZV2P;
- ➢ Ecut rho = 280.0 Ry;
- ➢ Periodic Boundary Condition (PBC);
- ➢ Born-Oppenheimer molecular dynamics (BOMD) simulations (time step= 1 fs);
- ➢ NVT simulations.

Hydrogenated a-Si



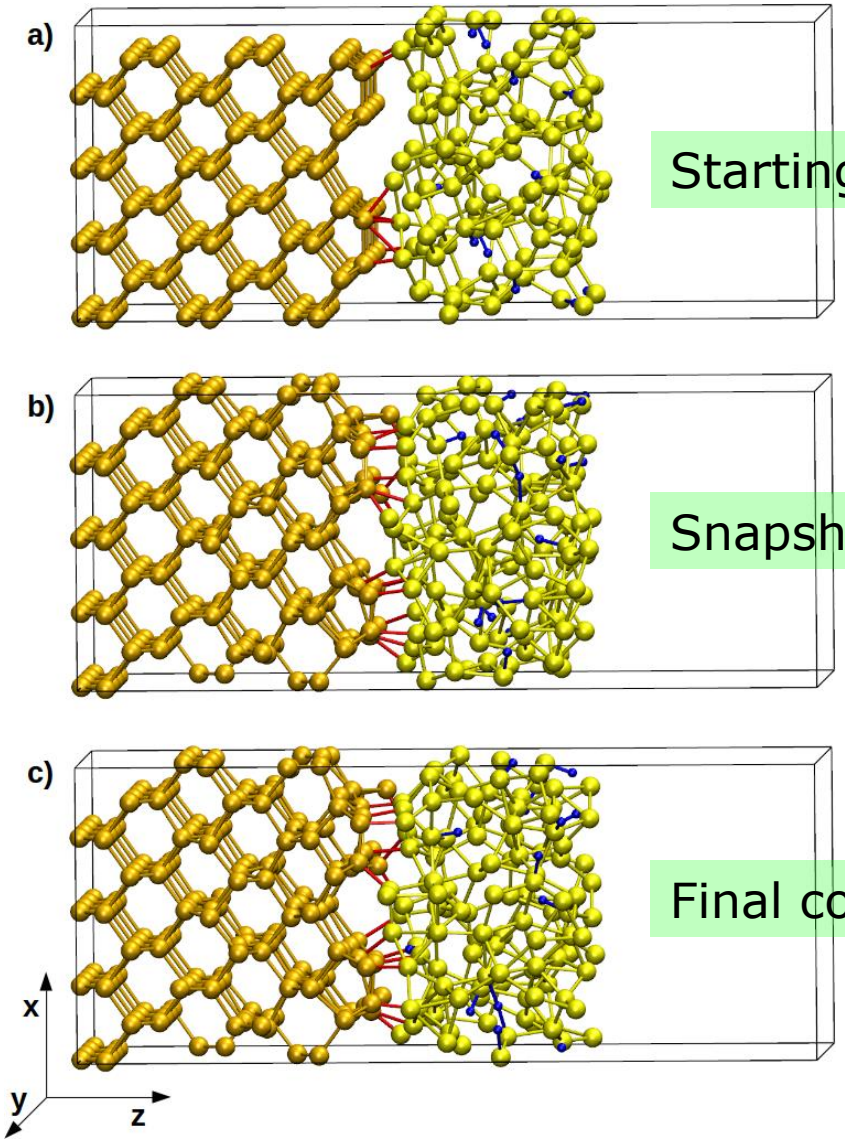
Coor.	n (%)	Env.	
1	0	Si1H0	0
2	0	Si2H0 Si1H1	0 0
3	4 (0.8)	Si3H0 Si2H1	4 0
4	507 (99.0)	Si4H0 Si3H1 Si2H2	443 64 0
5	1 (0.2)	Si5H0 Si4H1 Si5H2	1 0 0

Peaks at 1.51 Å (Si-H) and 2.37 Å (Si-Si)



Curioni et al. Large-scale simulations of a-Si:H: the origin of midgap states revisited. Phys. Rev. Lett. 107 (2011) 255502.
Laaziri et al. High resolution radial distribution function of pure amorphous silicon. Phys. Rev. Lett. 82 (1999) 3460.

c-Si/a-Si:H interface



Starting configuration

Snapshot at 25 ps

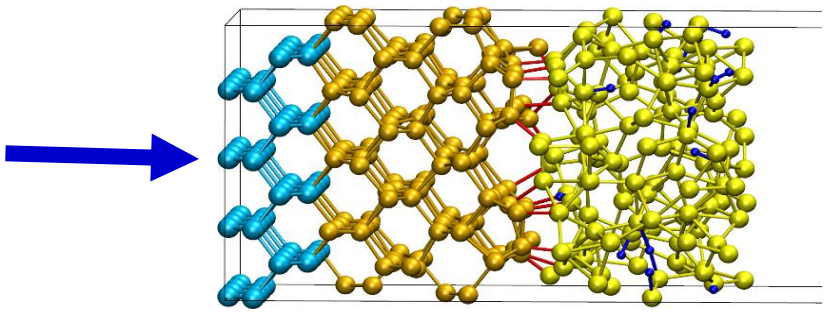
Final configuration at 35 ps

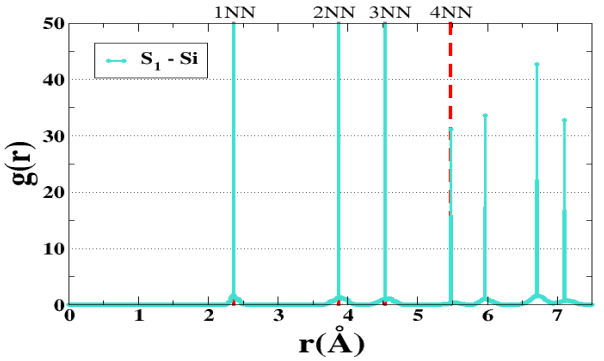
cSi aSi H

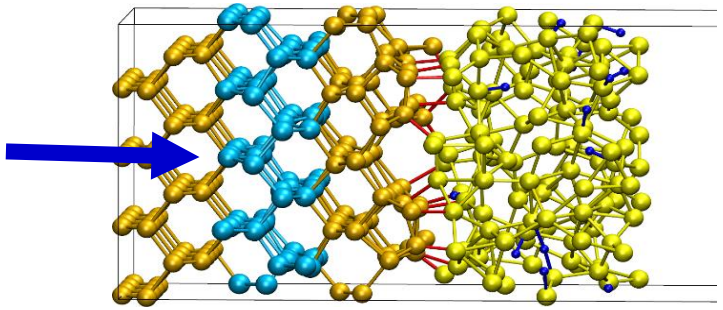
- Tetragonal cell
- Lx = Ly = 15.46 Å; Lz =38.66 Å
- 10 Å void
- 336 atoms (320 Si + 16 H)
- c-Si side 192 Si
- a-Si:H side 128 Si + 16 H
- BOMD at 300 K
- t = 35 ps

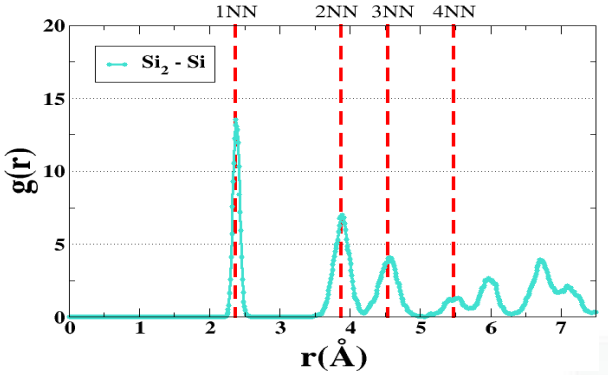
c-Si/a-Si:H interface

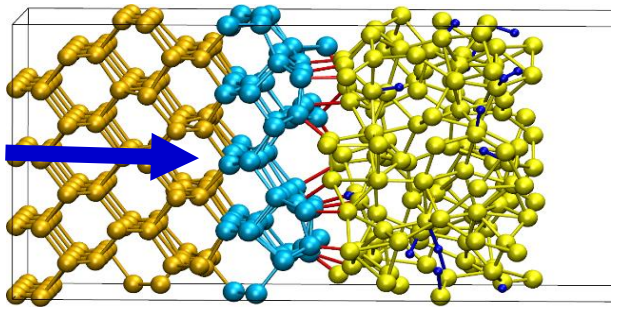
Pair correlation function g(r) computed on three slices of the crystalline part c-Si

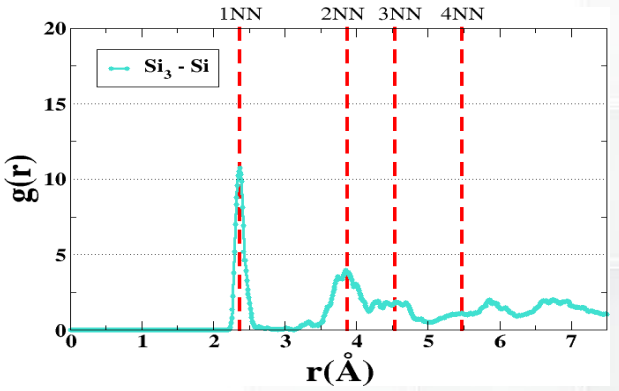






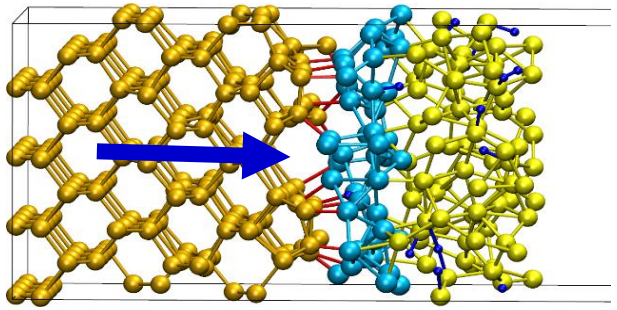


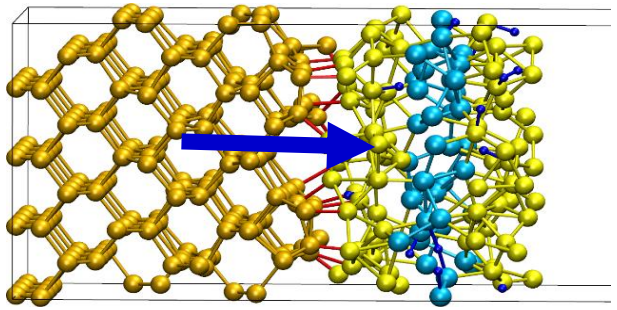


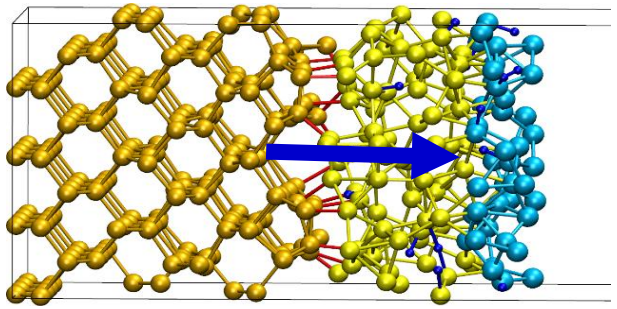


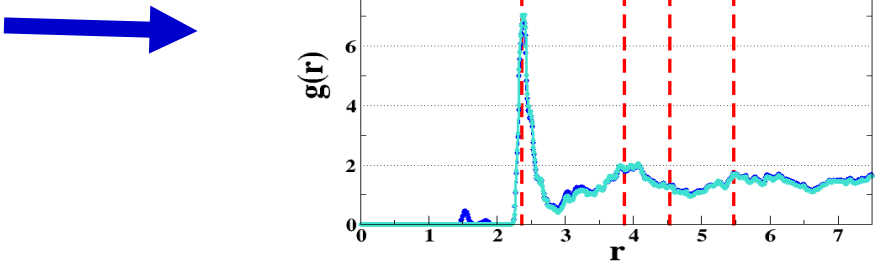
c-Si/a-Si:H interface

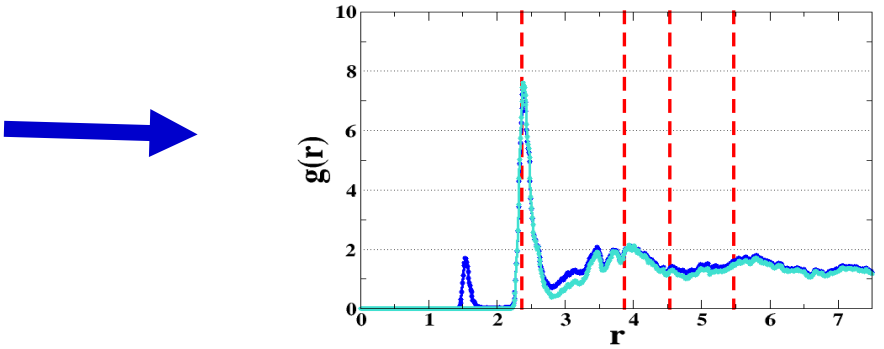
Pair correlation function g(r) computed on three slices of the amorphous part a-Si:H

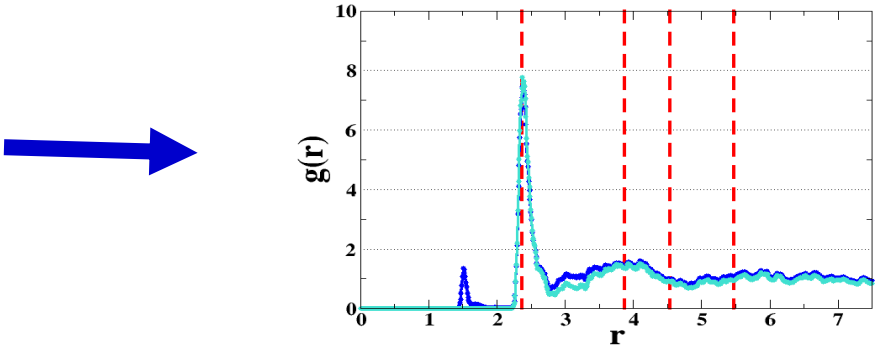






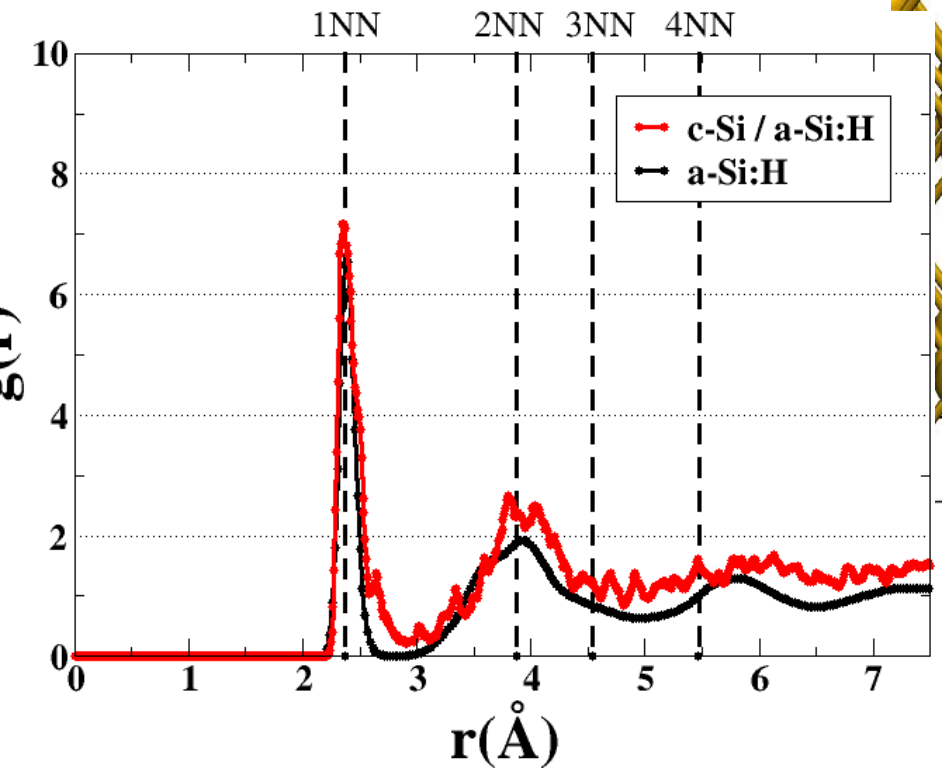


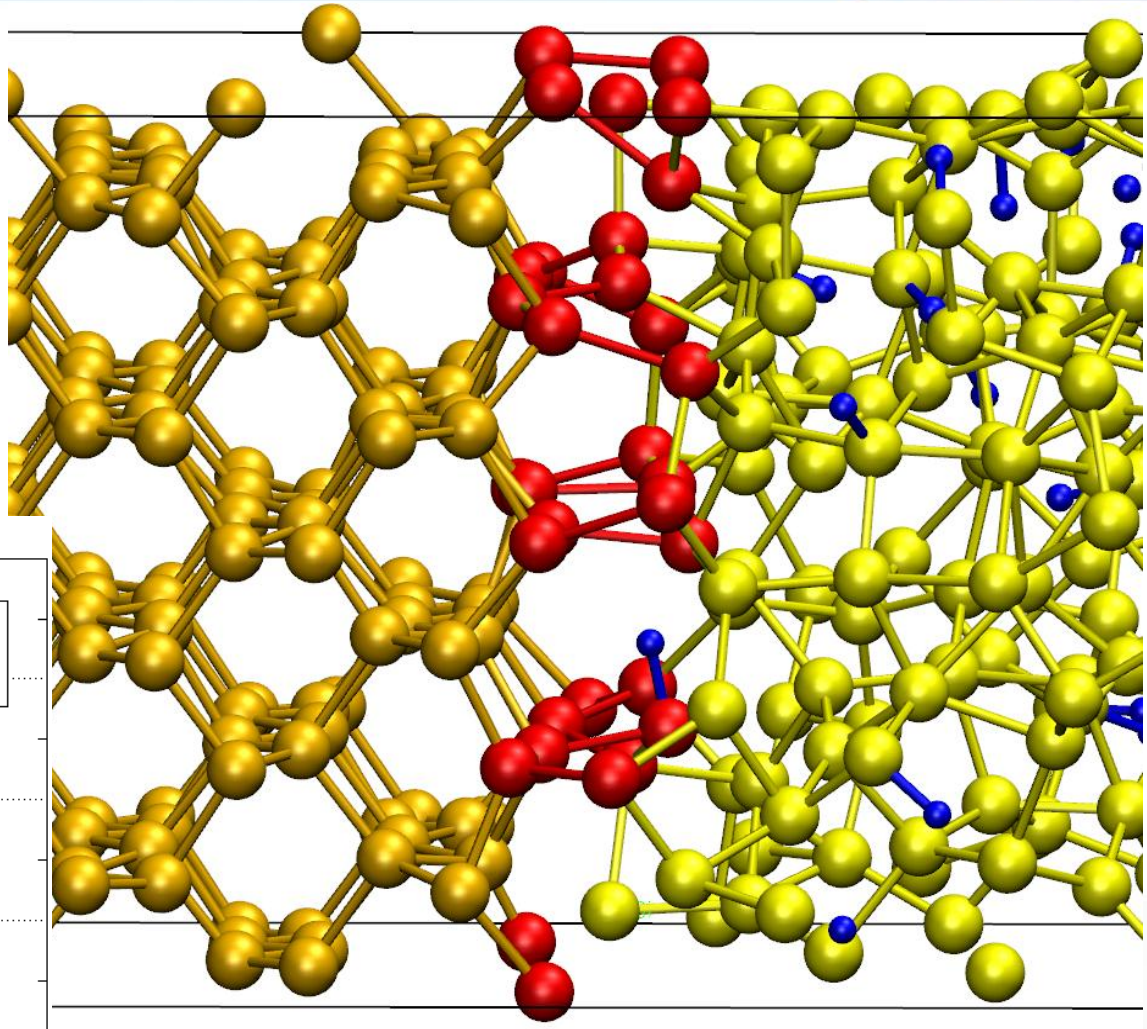




c-Si/a-Si:H interface

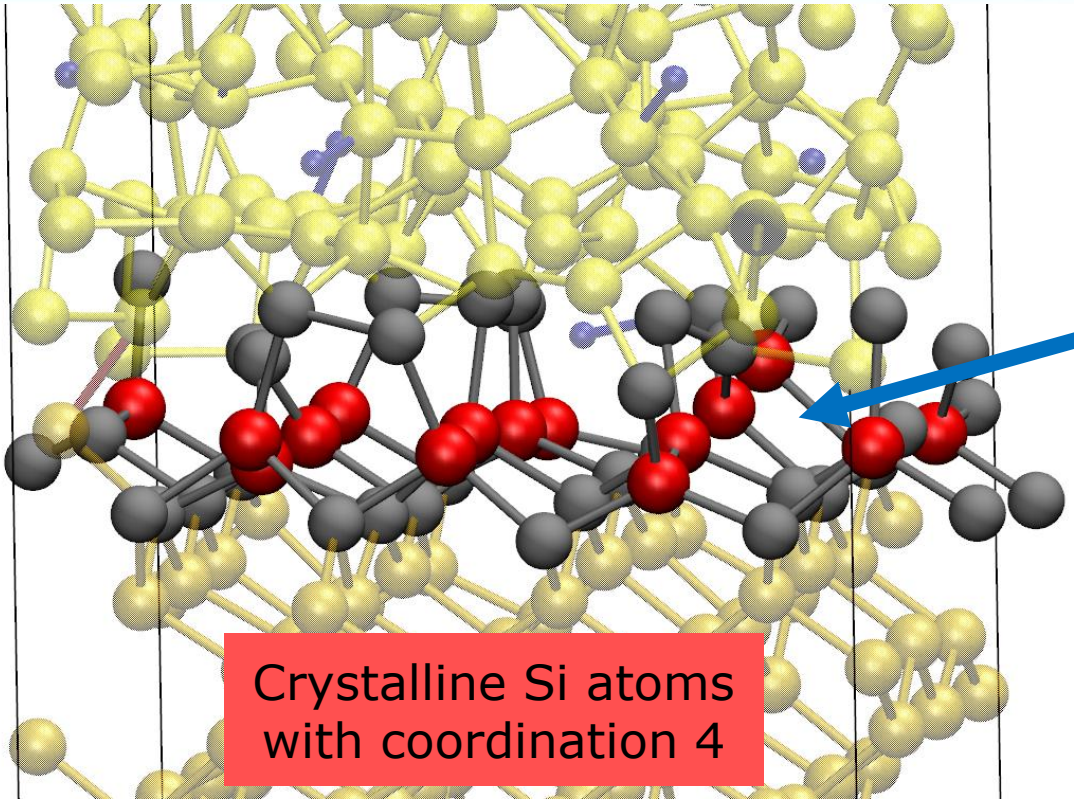
Pair correlation function computed on the red atoms at the interface





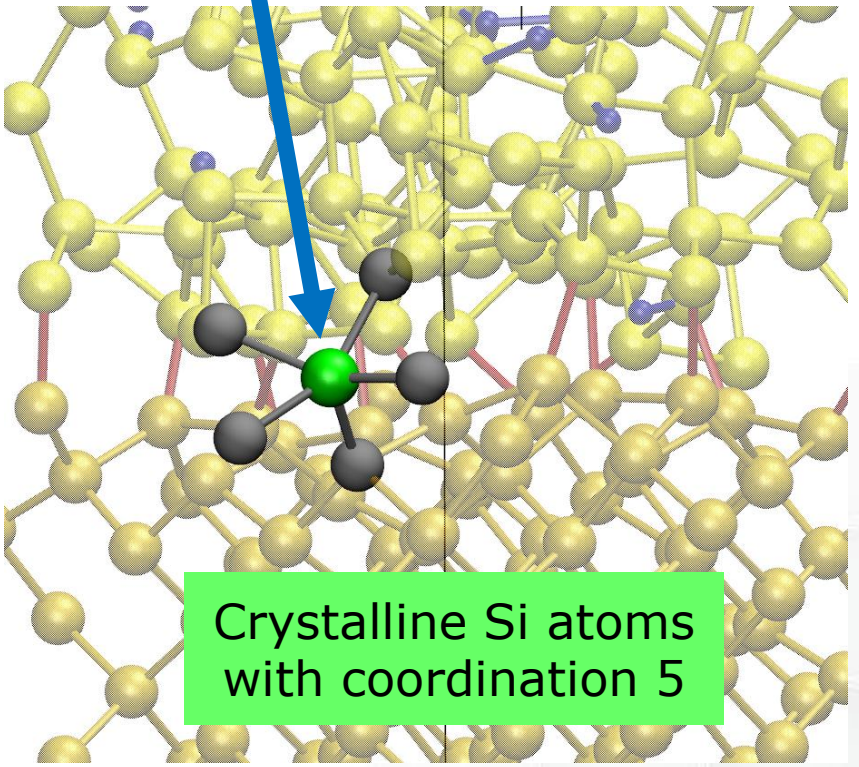
Red atoms are couples formed by 1 c-Si atom and 1 a-Si atom with distance < 2.9 Å
16 couples

c-Si/a-Si:H interface



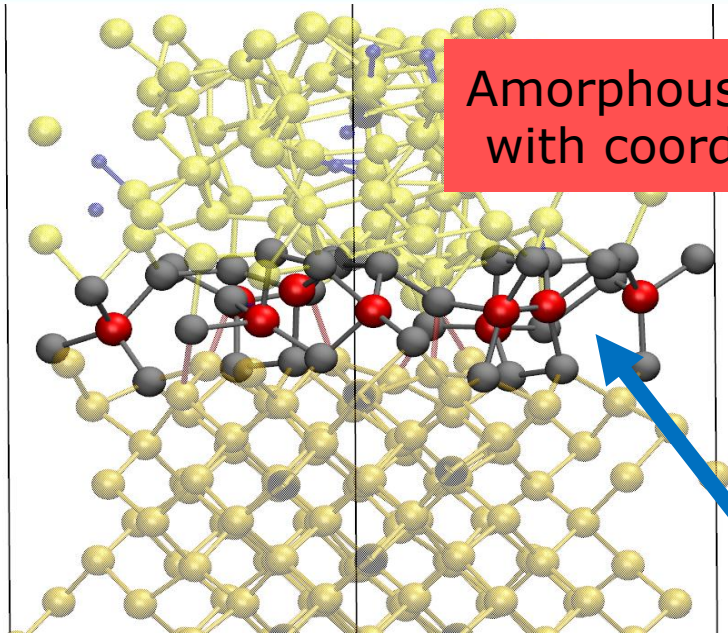
Crystalline Si atoms with coordination 4

Coor.	n	Env.
4	15	Si4H0
5	1	Si5H0

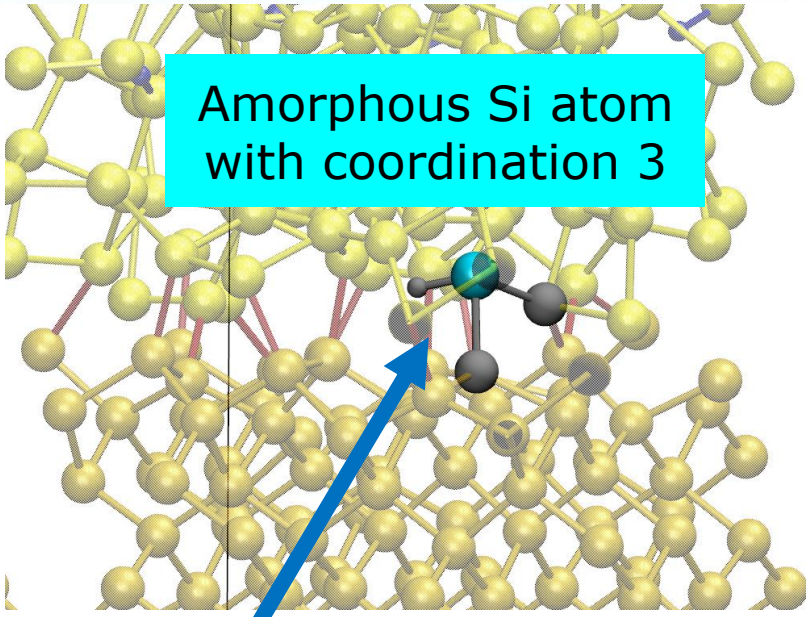


Crystalline Si atoms with coordination 5

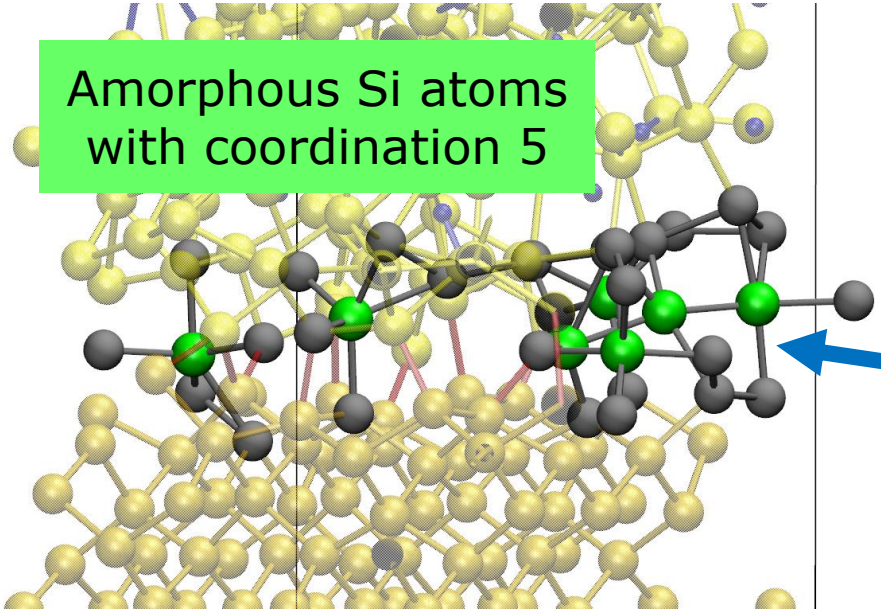
c-Si/a-Si:H interface



Amorphous Si atoms with coordination 4



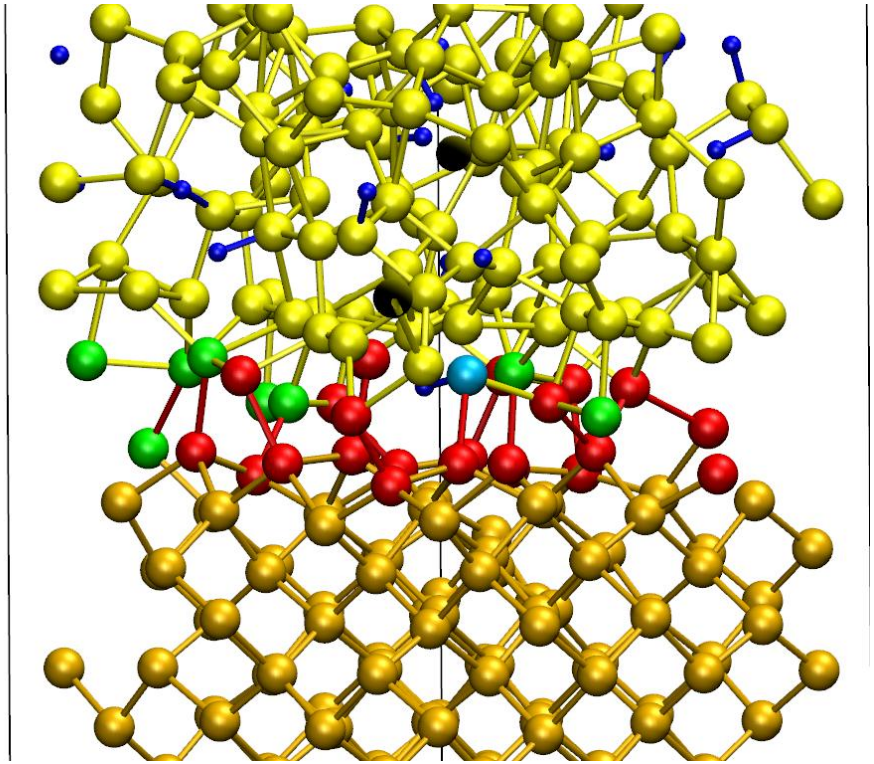
Amorphous Si atom with coordination 3



Amorphous Si atoms with coordination 5

Coor.	n	Env.
3	1	Si2H1
4	9	Si4H0
5	7	Si5H0

c-Si/a-Si:H interface



Si atom with coordination 3

Si atoms with coordination 4

Si atoms with coordination 5

We characterized the Silicon based materials, in particular a-Si:H and c-Si/a-Si:H, performing MD and analysing the structural properties.
Our colleagues are using these configurations to calculate the electronic structure (ELF, DOS, spread) and to have a better insight on these systems.

Thanks for your attention