# ENEA partnership in the European Energy oriented Centre of Excellence (EoCoE )

F. Ambrosino, G. Bracco, F. Buonocore, M. Celino, A. Colavincenzo, A. Funel, S. Giusepponi, G. Guarnieri, M. Gusso, S. Migliori, G. Ponti, A. Quintiliani

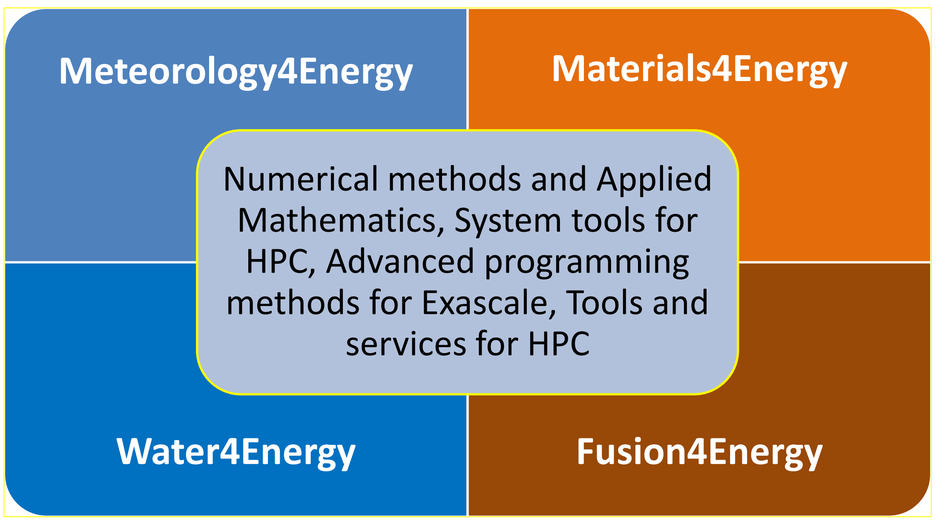
Energy Technologies Department
ICT Division

## The European Energy oriented Centre of Excellence in computing applications

EoCoE (read as “Echo”) has been funded from 2015 to 2018 to exploit the tremendous potential offered by the HPC computing infrastructures to foster and accelerate the European transition to a reliable low carbon energy.

Coordinator: Prof. Edouard Audit (Maison De La Simulation, CEA Saclay). Franco-German hub coordinating a pan-European network in which partners are strongly engaged in both HPC and energy fields (21 partners , 8 countries)


**EoCoE 2 !!**
**2019- 2021**




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.

www.eocoe.eu

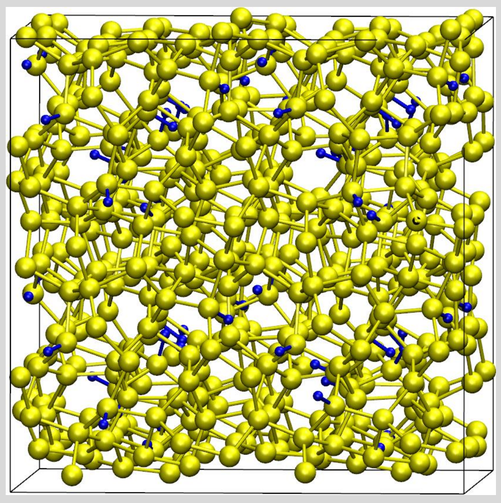
Horizon 2020
European Union funding
for Research & Innovation

European Commission

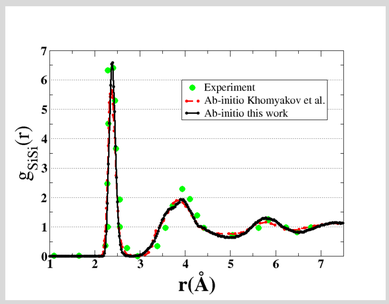
## Interface modeling for heterojunctions solar cells applications

Partnership with
U. Aeberhard and P. Czaja
JÜLICH FORSCHUNGSZENTRUM

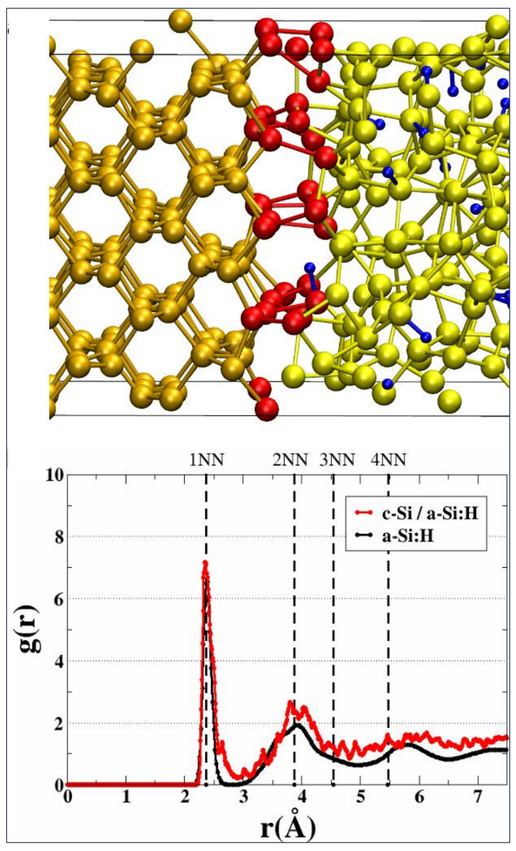
The atomic and electronic structure at the amorphous hydrogenated silicon is the starting point for the design of a crystalline Si – hydrogenated amorphous Si interface.

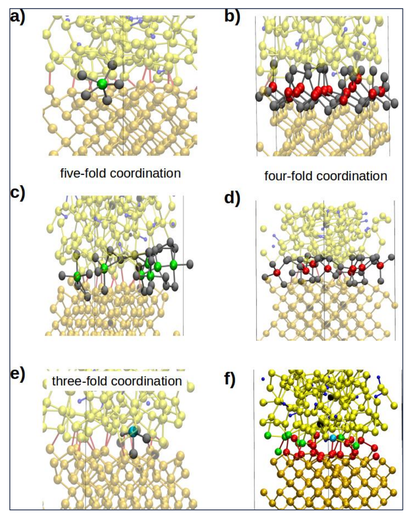


Very good agreement with the experimental structure




**Atomic scale design of the interface to reduce structural and chemical defects**



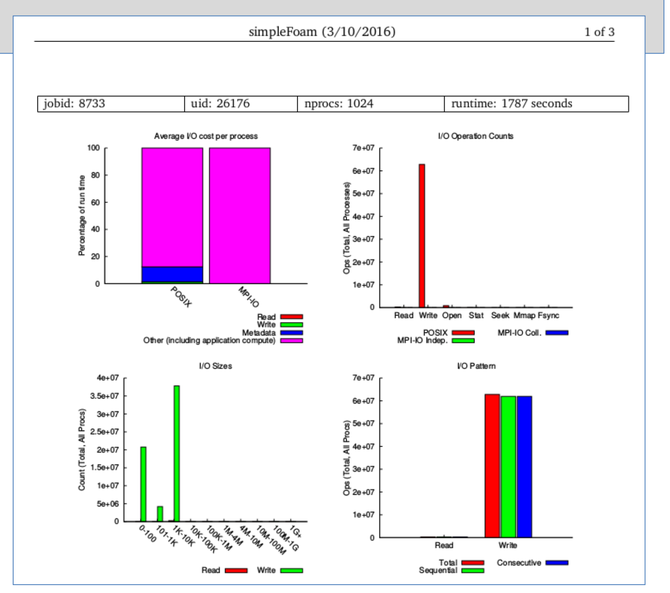

Coordination and electronic analysis of the interface

More information on the Computational Materials Science and Technology Virtual Lab webpage: www.afs.enea.it/project/cmast

## The I/O benchmarking methodology of EoCoE project

An efficient I/O is crucial for a fast execution of a code. Often the bottleneck is due to poor I/O performances. There are many causes which may degrade I/O performances: inefficient I/O strategy, inappropriate size of I/O buffers, large number of I/O calls, poor file system performances etc. It is very important to use benchmarks to get I/O behaviour in a reproducible way to identify and remove bottlenecks. The adopted methodology is outlined below: measure I/O pattern at runtime (Darshan) [1], simulate the I/O pattern on many HPC systems to find bottlenecks (IOR) [2], remove bottlenecks.

Example of I/O pattern captured by Darshan for a CFD (external aerodynamics) simulation on CRESCO4 [3] supercomputer at ENEA [4]. CRESCO4 system has ~300 nodes each of which with 2x8 cores Intel Sandy Bridge (E5-2670 2.6 GHz) 64 GB RAM. The simulation used 1024 cores and a GPFS file system with 6 I/O servers over IB 4xQDR (40 Gbps) network. The run execution time was ~1420 s. This example shows that the huge number of I/O accesses (~830000) and the small I/O size (~KB) are hints for a bottleneck.




[1] http://www.mcs.anl.gov/research/projects/darshan/
[2] https://github.com/LLNL/ior
[3] http://www.cresco.enea.it/
[4] http://www.enea.it/it