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

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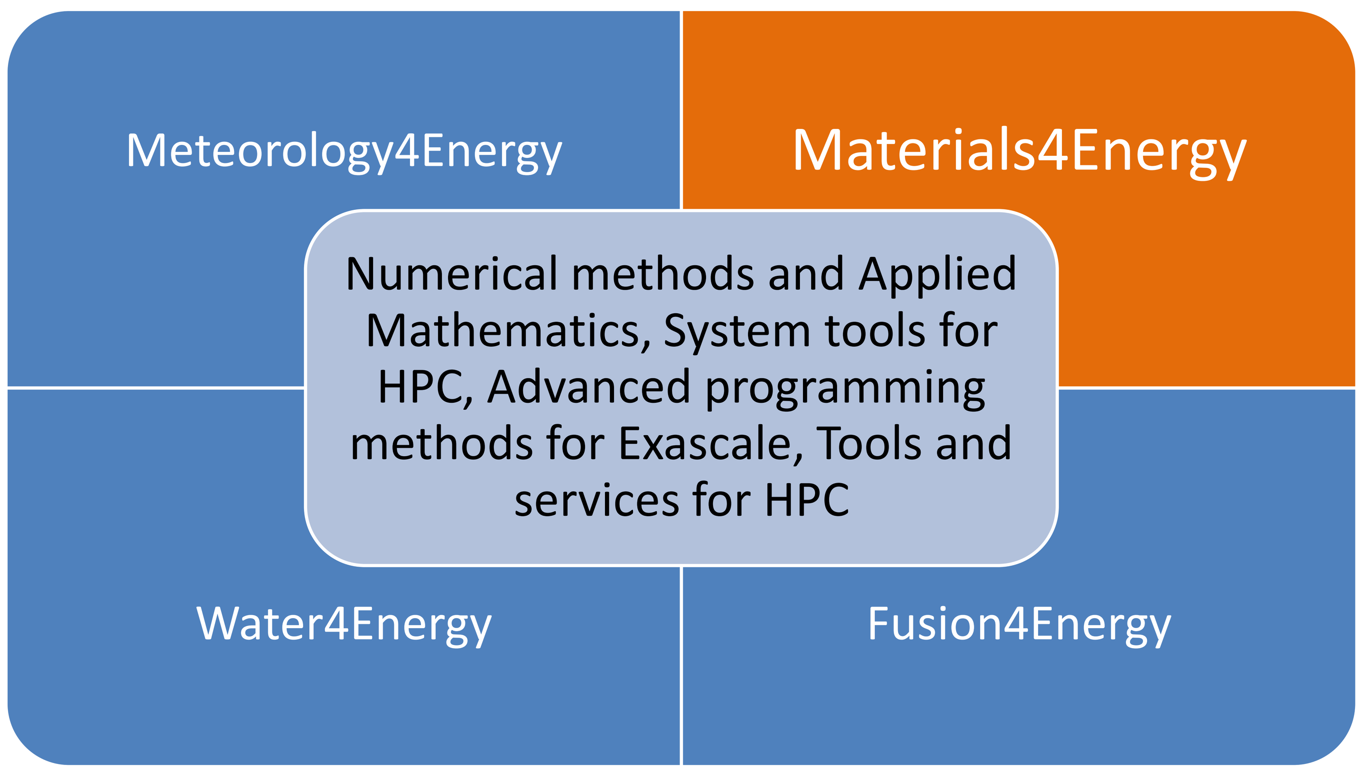
The European Energy oriented Centre of Excellence in computing applications

EoCoE (read as "Echo") uses the tremendous potential offered by the ever-growing computing infrastructure to foster and accelerate the European transition to a reliable low carbon energy supply using HPC (High Performance Computing).

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)



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
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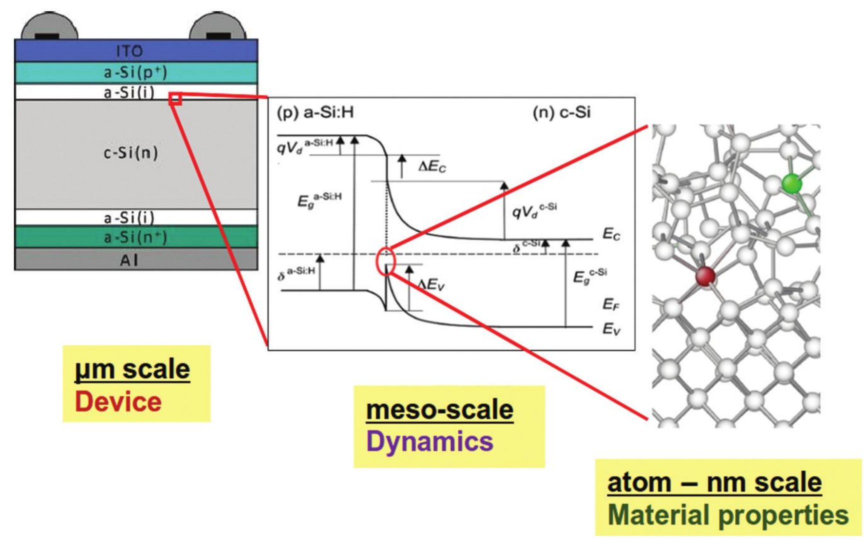
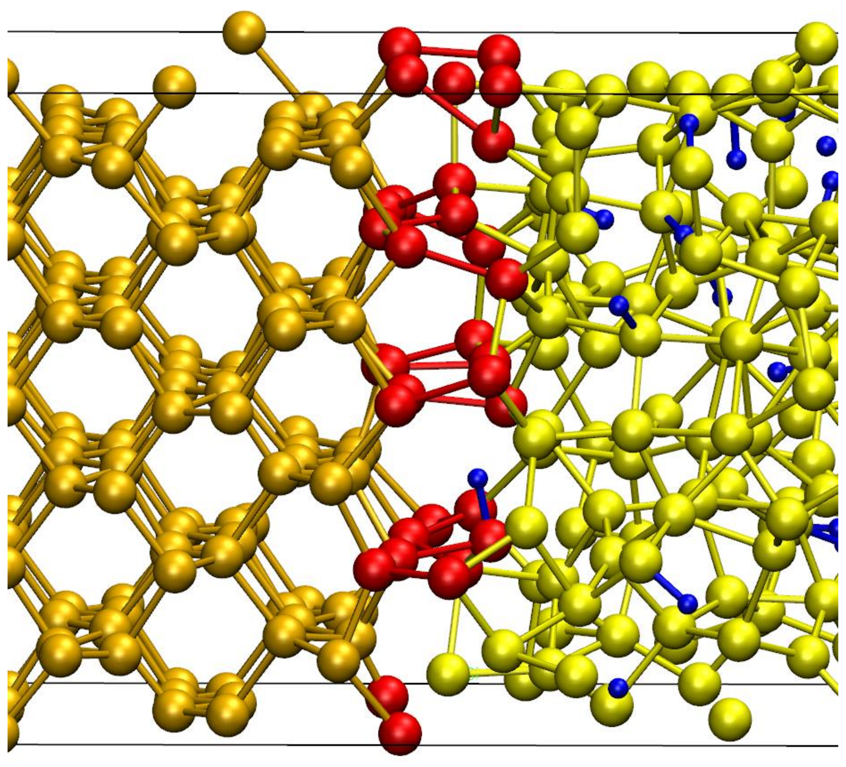
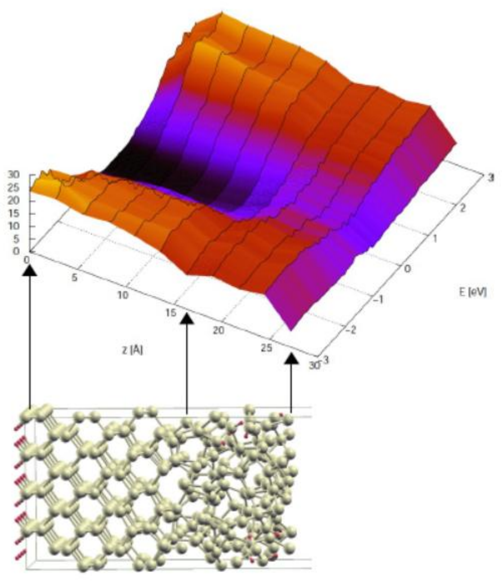
Multiscale modeling of heterojunctions solar cells



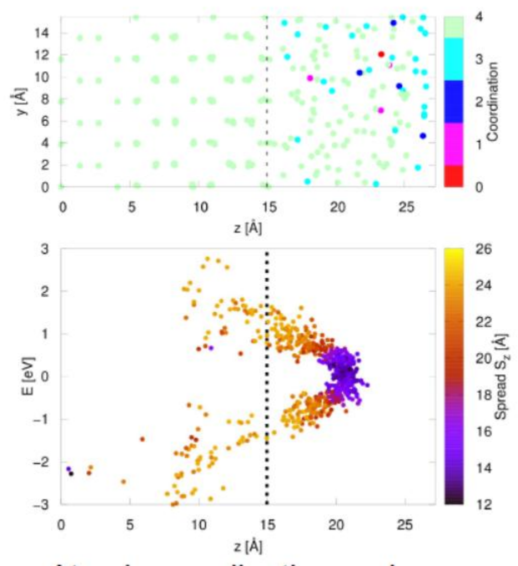
Multi-scale scheme for the electronic simulation of SHJ devices to propagate local material properties at the interface via meso-scale charge carrier dynamics in the heterojunction region to performance relevant features in the global device characteristics.

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.





Layer-resolved DOS



Atomic coordination and localization of wave functions in different regions of the interface

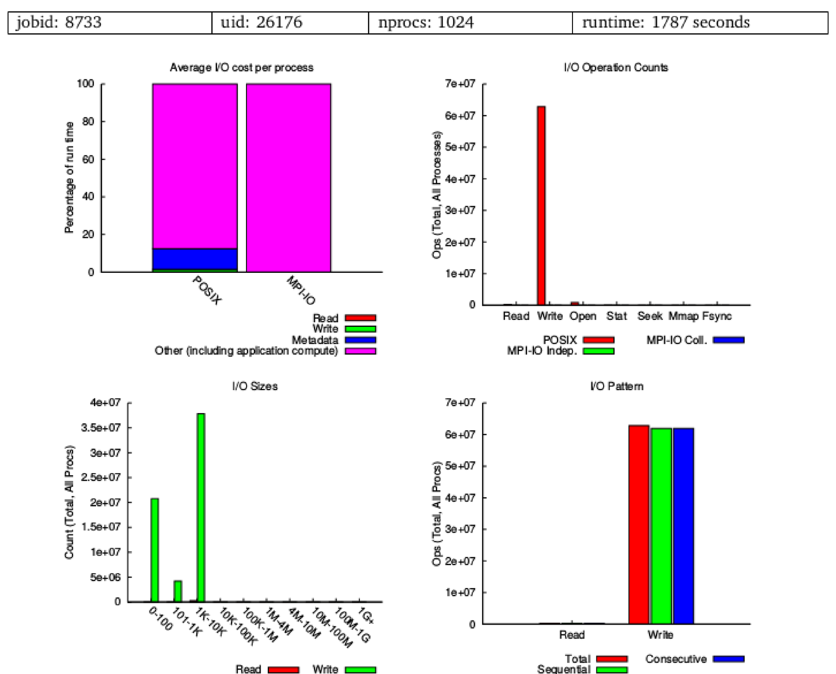
More information in the Computational Materials Science and Technology Virtual Lab webpage www.afs.enea.it/project/cmast

The I/O benchmarking methodology of EoCoE project

An efficient I/O is crucial for a fast execution of a code. It could happen that a code run fast on a HPC platform and slow on another even if the two systems have the same microprocessor. 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:

- find I/O pattern at runtime (Darshan) [1]
- simulate the I/O pattern on many HPC systems to find bottlenecks (IOR) [2]
-remove bottlenecks:
  - code changes,
  - optimized libraries,
  - code refactoring
  - integration of optimized libraries

[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



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.