QUANTUMESPRESSO

Quantum ESPRESSO is an **open-source** suite of computer codes that implements state-of-the-art electronic-structure methods for **materials modelling** at the atomic/nano-scale.

QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials
Author(s): Giannozzi, P; Baroni, S; Bonini, N, et al.

JOURNAL OF PHYSICS-CONDENSED MATTER
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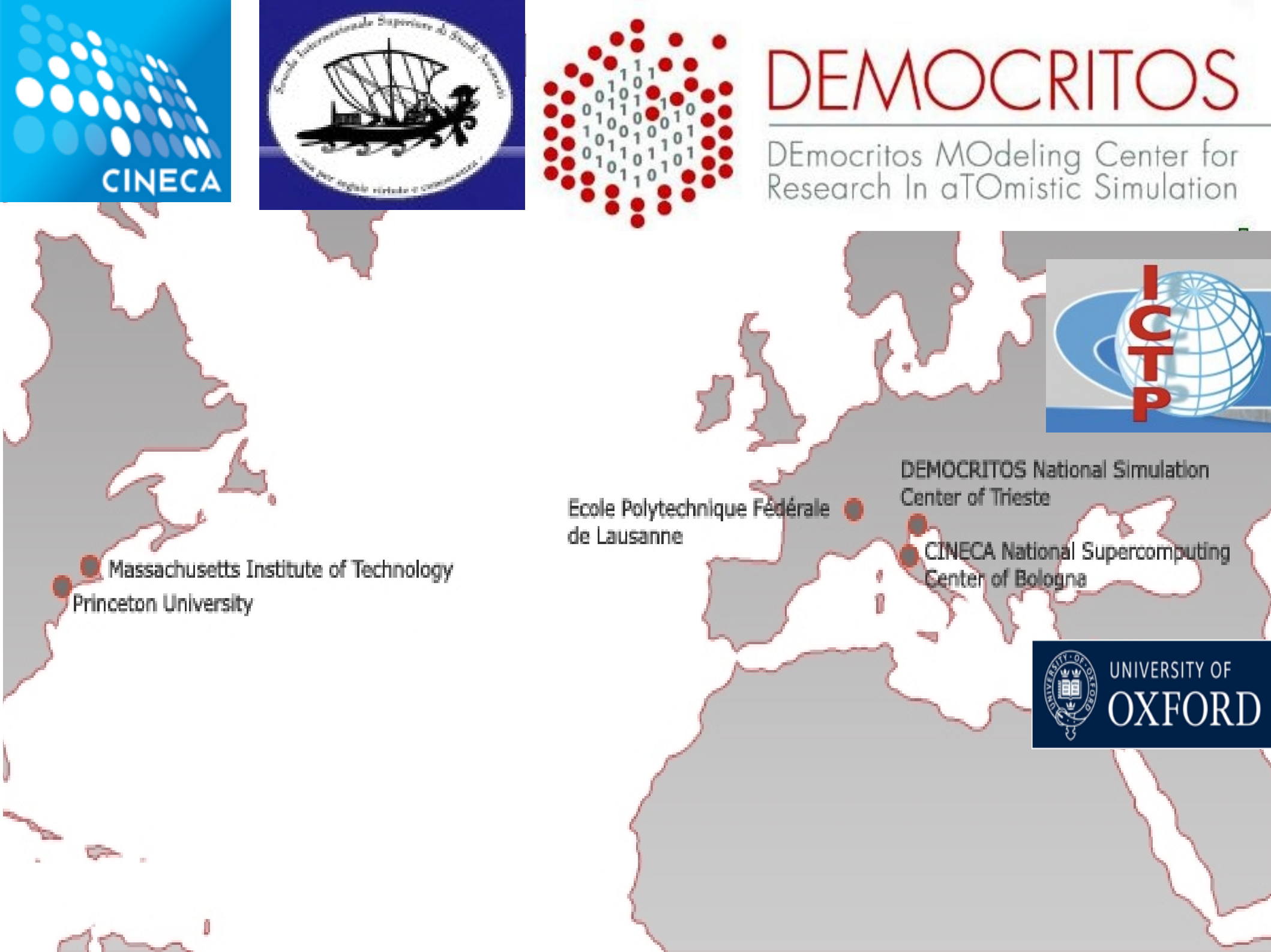
www.quantum-espresso.org


CINECA
DEMOCRITOS
DEmocritos MOdeling Center for
Research In aTOmistic Simulation
ICTP
DEMOCRITOS National Simulation
Center of Trieste
Ecole Polytechnique Fédérale
de Lausanne
CINECA National Supercomputing
Center of Bologna
Massachusetts Institute of Technology
Princeton University
UNIVERSITY OF
OXFORD

Material modelling

Questions that one would like to answer ...

- Why some material has a particular behavior?
- Would some material exhibit some particular property?
- Would this material work if submitted to ... ?
- Which material/materials do I have in my sample?

without the need of making experiments or going beyond the experimental sensitivity

Steps

- Finding of the equilibrium structure (ions and electrons)
- “Post-processing”:
  - STM images
  - Density of States
  - plot of the electronic density and/or states
  - Absorption spectra
  - etc

FEATURES

espresso-4.1

- Structure optimisation
- Phonons
- Elastic constants
- Quantum transport
- Ab-initio molecular dynamics
- Dielectric and Raman tensors
- Infrared spectra
- NMR spectra
- ...

access to development version is open

- Electronic excitations: absorption spectra, ionisation potentials, electron affinities
- Distributed together:
  - Quantum transport WanT

    www.want-code.org
  - Electronic excitations YAMBO

    www.yambo-code.org
  - coming soon Free energy reaction paths PLUMED

    http://merlino.mi.infn.it/~plumed/PLUMED/home.html

PERFORMANCES

ionic and electronic degree of freedom → big objects → relatively big communication between process

- Parallel computers : homogeneous architecture, fast communication between process → versatile

- Different parallelization levels
- Hybrid MPI-OPENMP

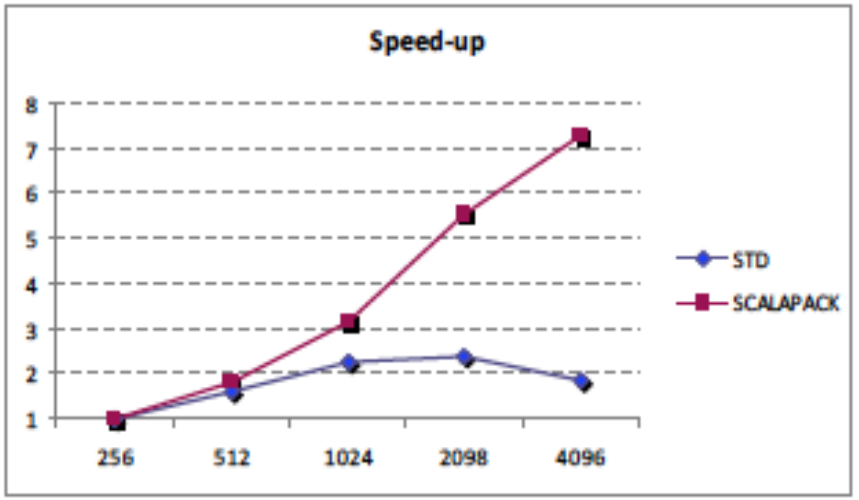
BENCHMARK CODE FOR:

Distributed
European
Infrastructure for
Supercomputing
Applications

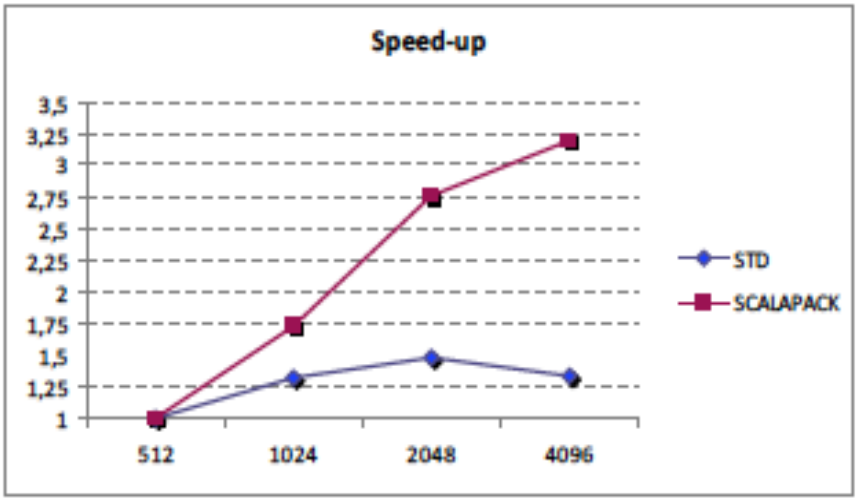
http://www.prace-project.eu/

scalable on thousand of procs

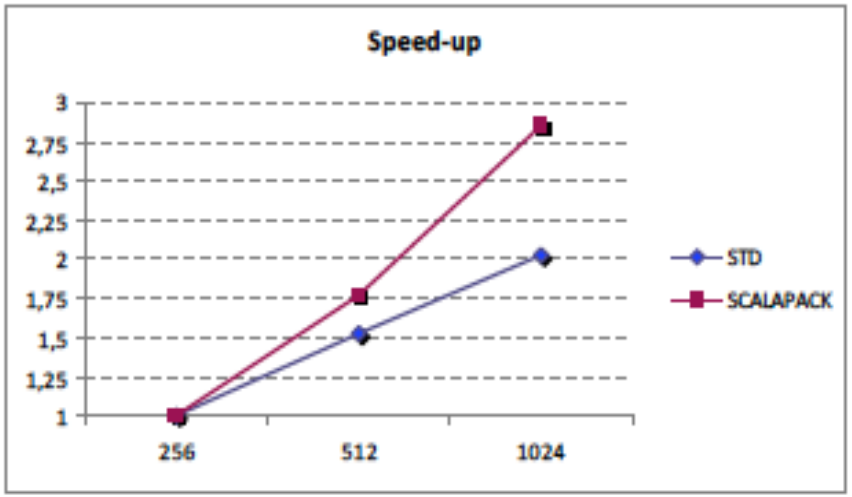
HECToR – PSIWAT (DEISA benchmark)



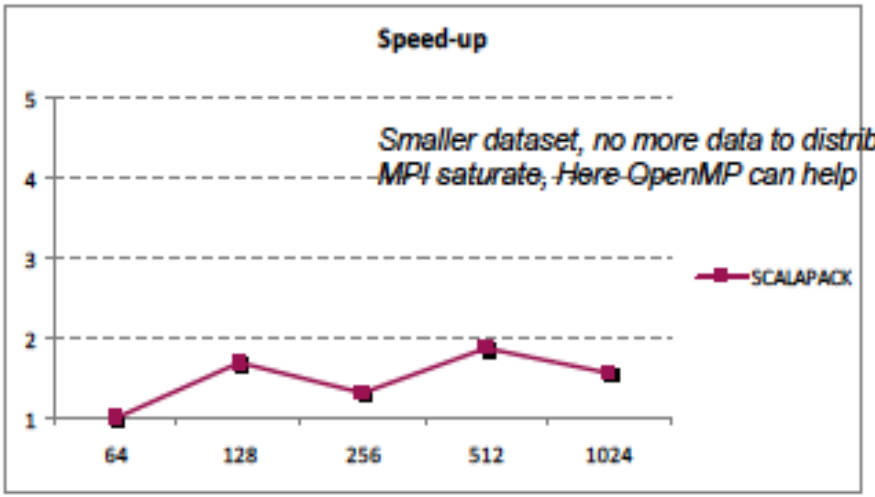
HECToR – CNT10POR8 (CINECA benchmark)



HPCx – PSIWAT (DEISA benchmark)



BCX – W256 (CINECA benchmark)

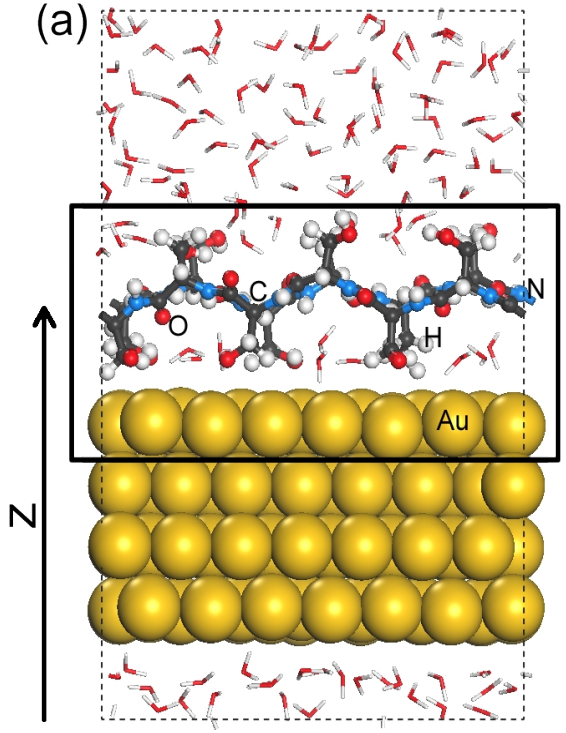


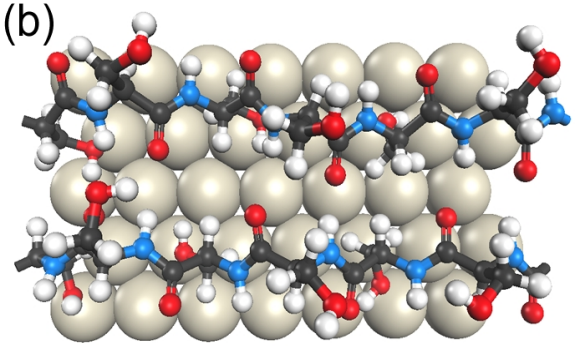
http://www.deisa.eu/science/benchmarking/results

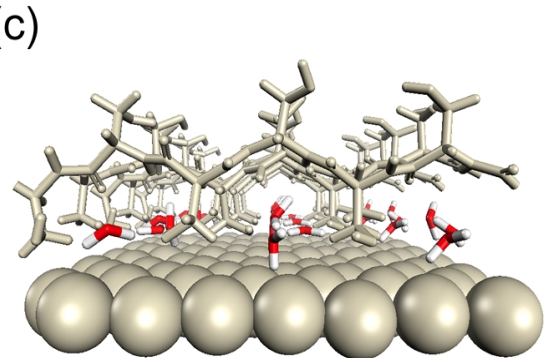
Courtesy of C. Cavazzoni,CINECA

EXAMPLES

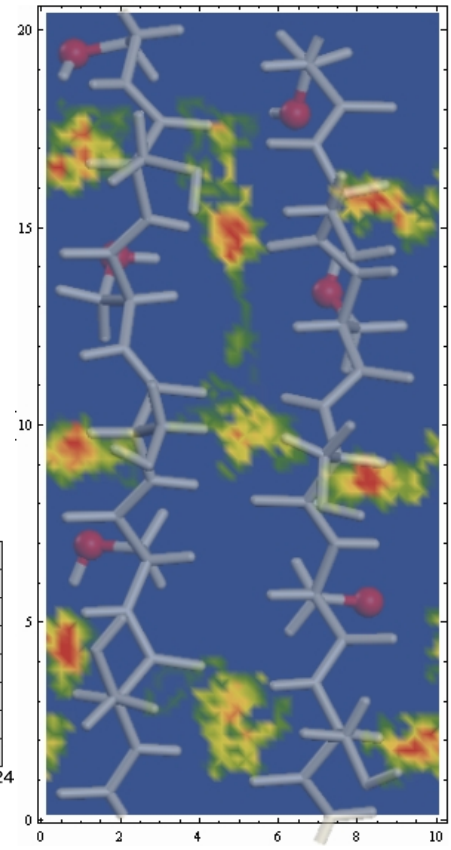
Ab-initio simulations of Protein-Surface Interactions mediated by WATer



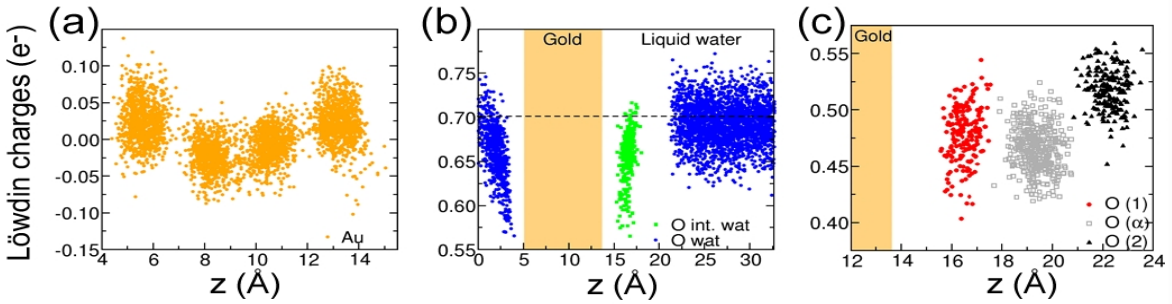




Density map of Oxygen in the hydration layers



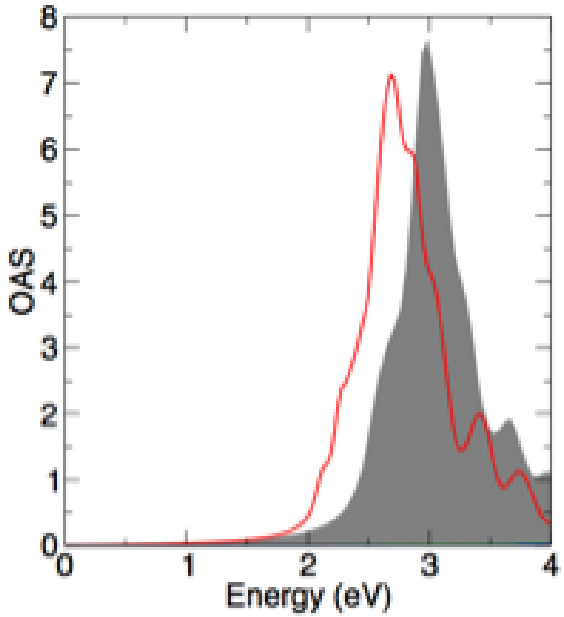
(a-c) Löwdin charges (dq) for selected atoms as a function of the positions, calculated with respect to the corresponding formal atomic values



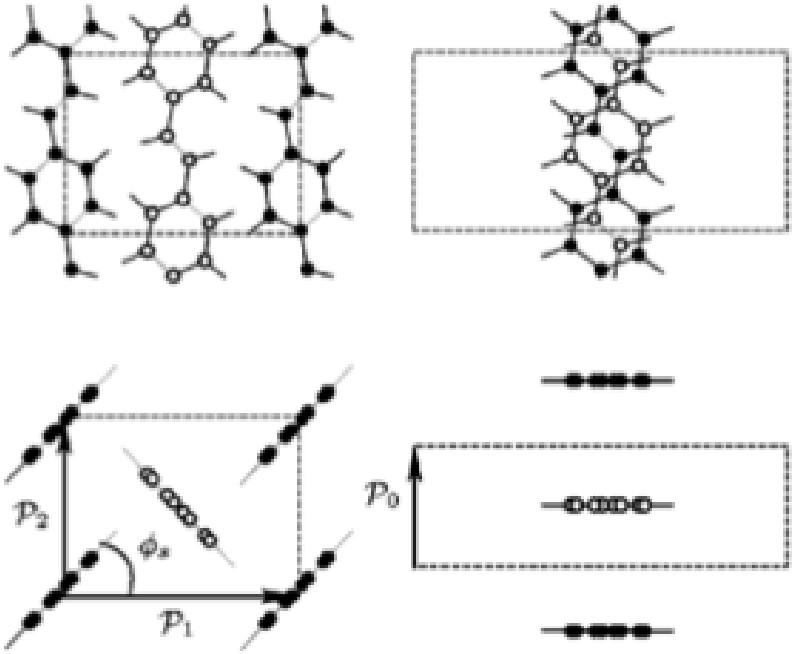
S. Corni, A. Calzolari, G. Cicero, C. Cavazzoni, A. Catellani and R. Di Felice

ElectroLuminescent Efficiency in polymers based Light Emitting Diodes

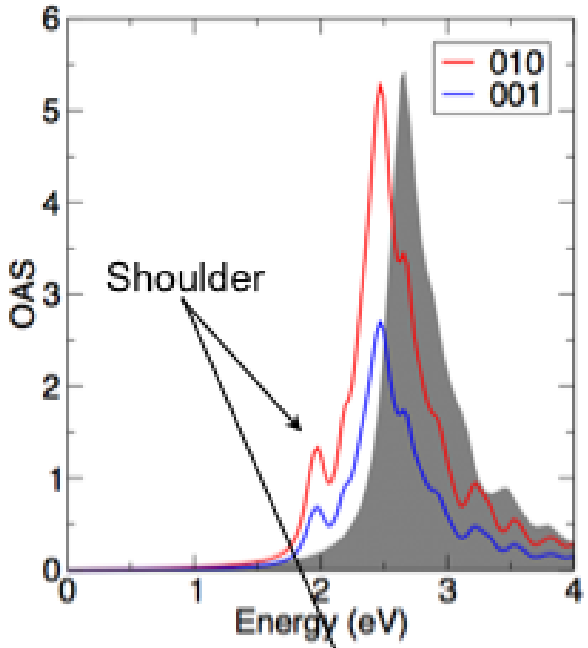
PPV as prototype polymer



Calculated optical absorption spectrum at 0K for HB-PPV

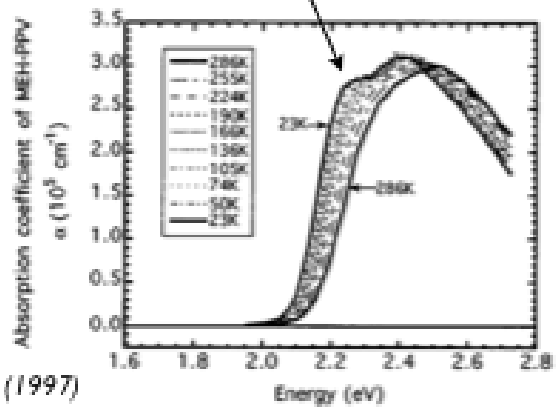


Calculated optical absorption spectrum at 0K for piS-PPV



Converged calculations: 8*runs of 48 hours, 192 procs of HLRB II (LRZ Munich, Germany)

Experimental optical absorption spectrum at different temperatures



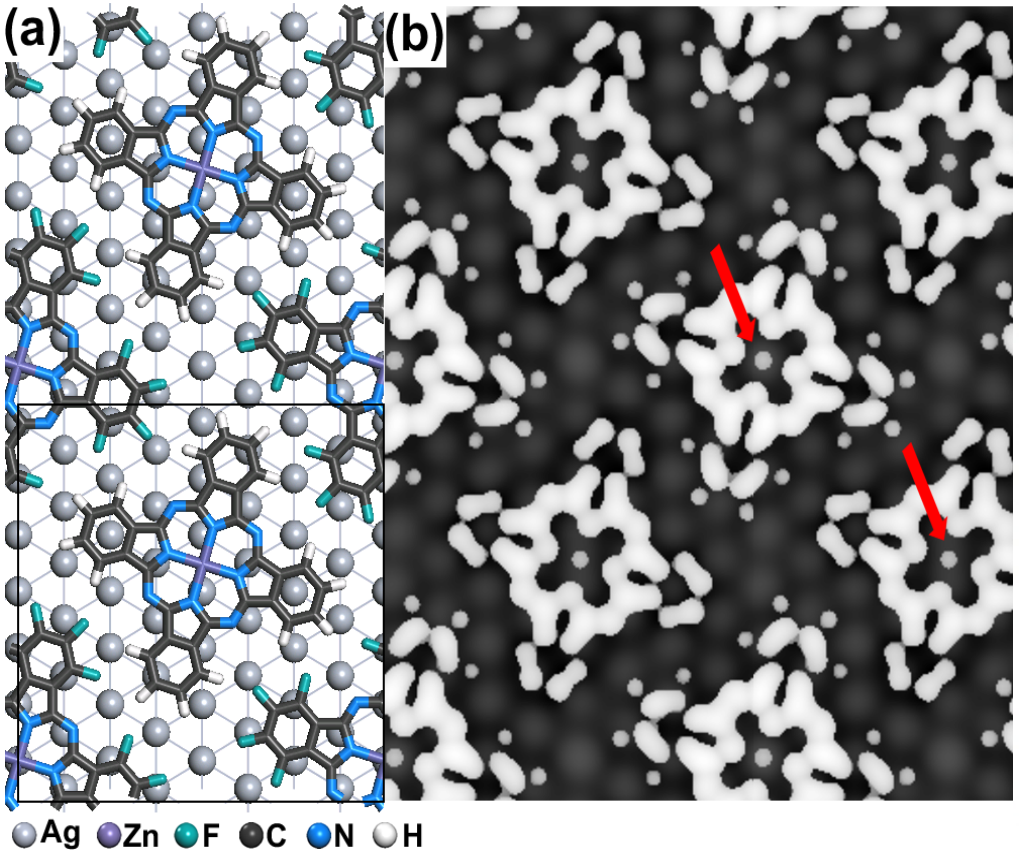
M.G. Harrison et al Phys. Rev. B 55, 7831 (1997)

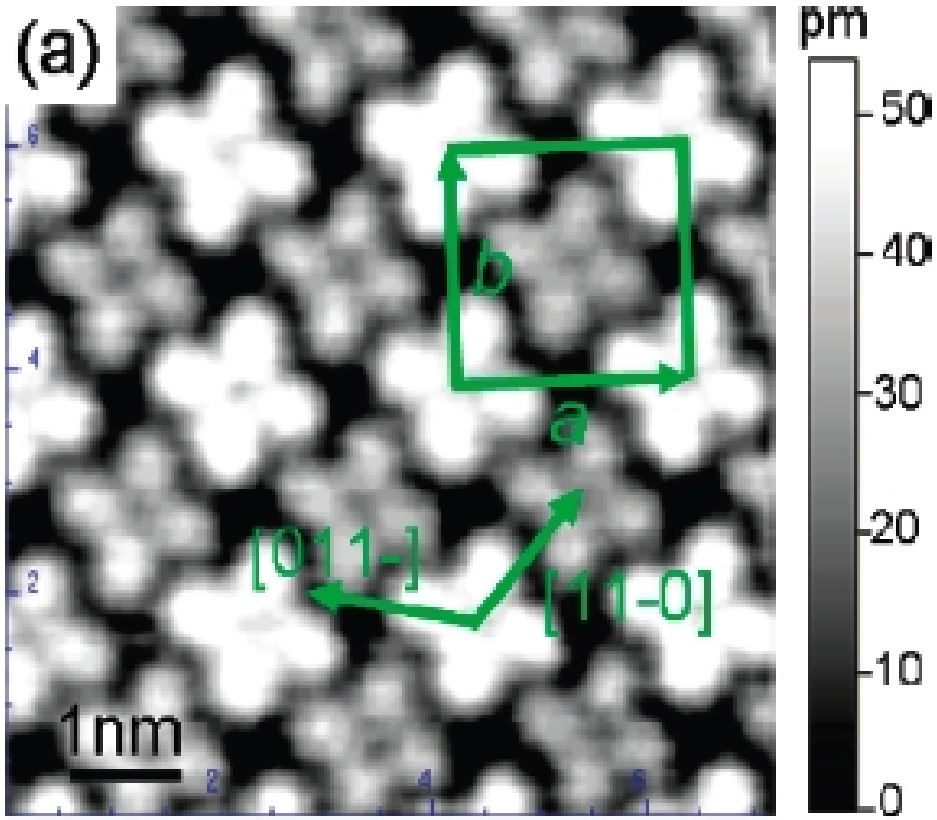
L. Martin-Samos, G. Bussi, A. Ruini, MJ Caldas and E. Molinari

Identification of surface equilibrium structures

Model

Experiment



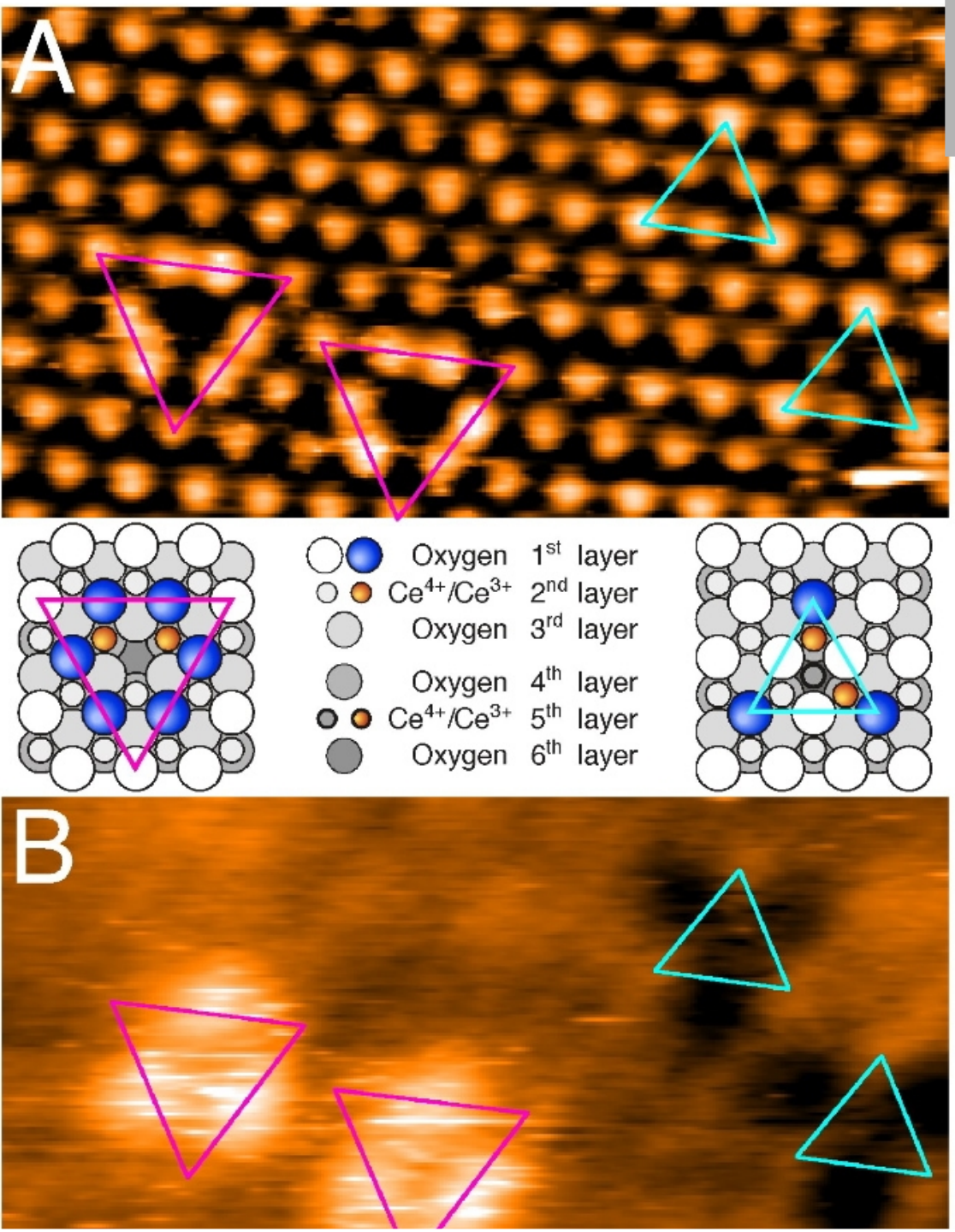


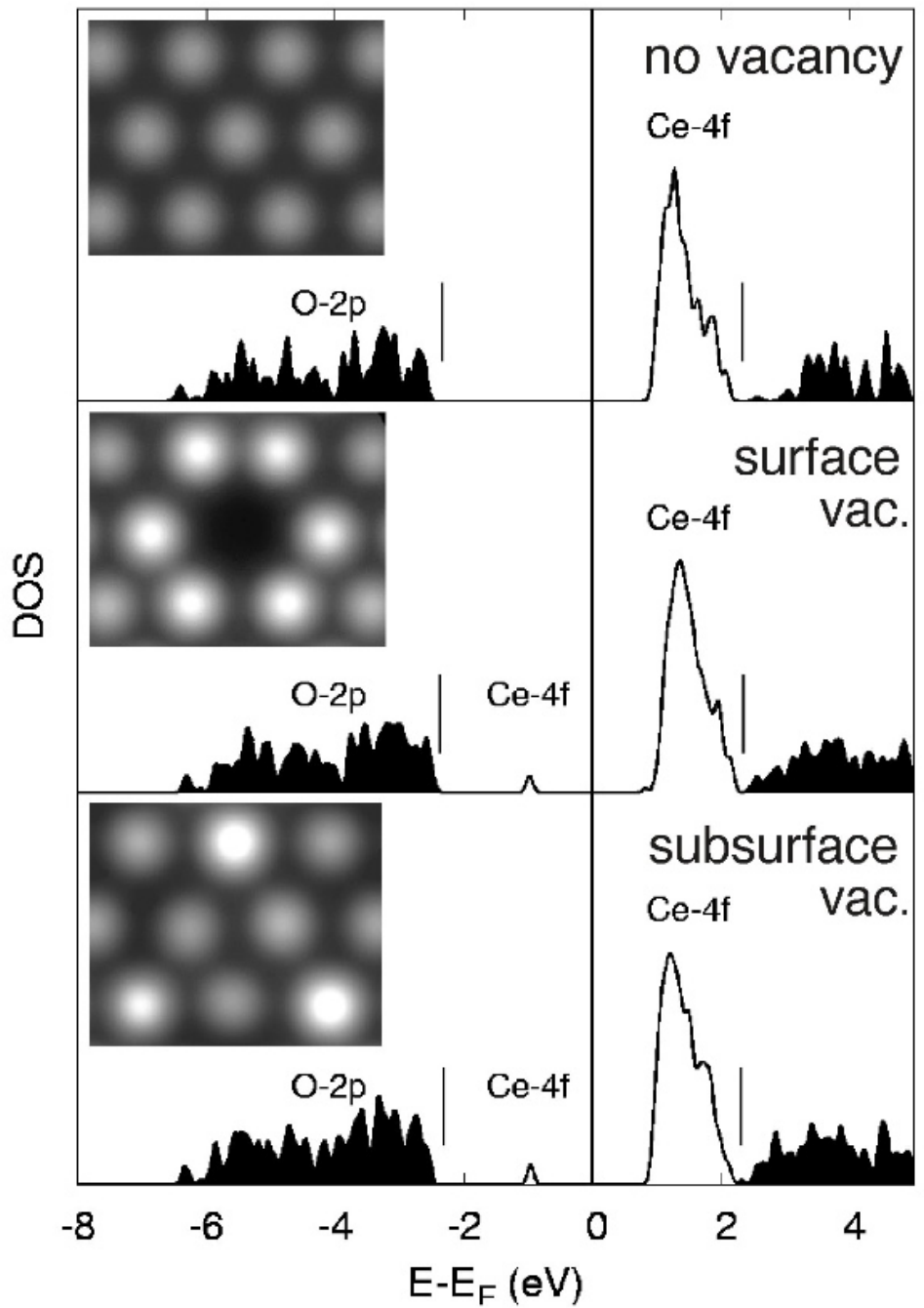
phthalocyanine + Zn or phthalocyanine+Fe16Zn
on Ag substrate

pw.x + pp.x

A. Calzolari, W. Jin, J. E. Reutt-Robey and M. Buongiorno Nardelli

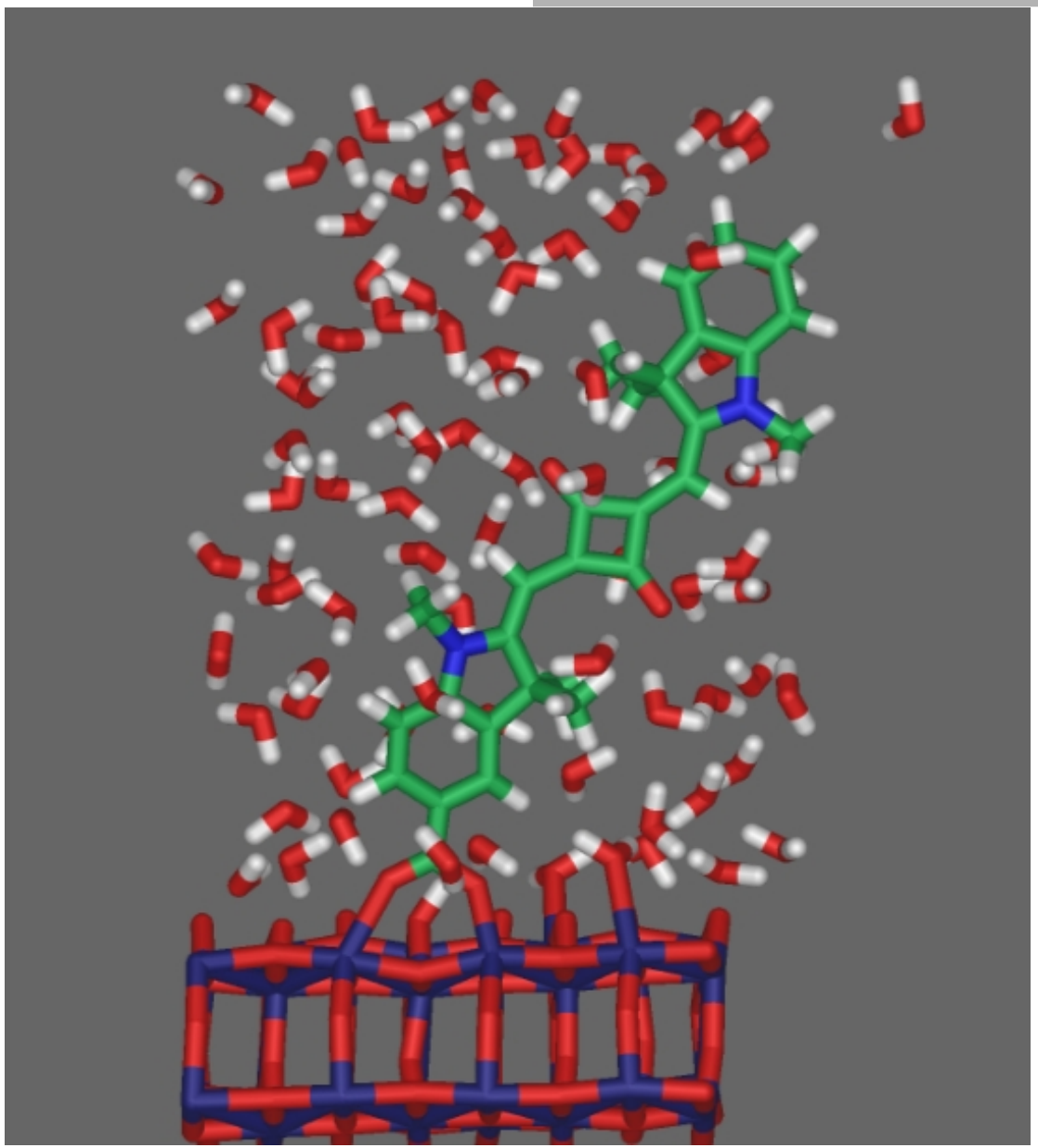
Identification of surface defects





F. Fabris *et al*

Solvated hybrid surfaces : equilibrium structure

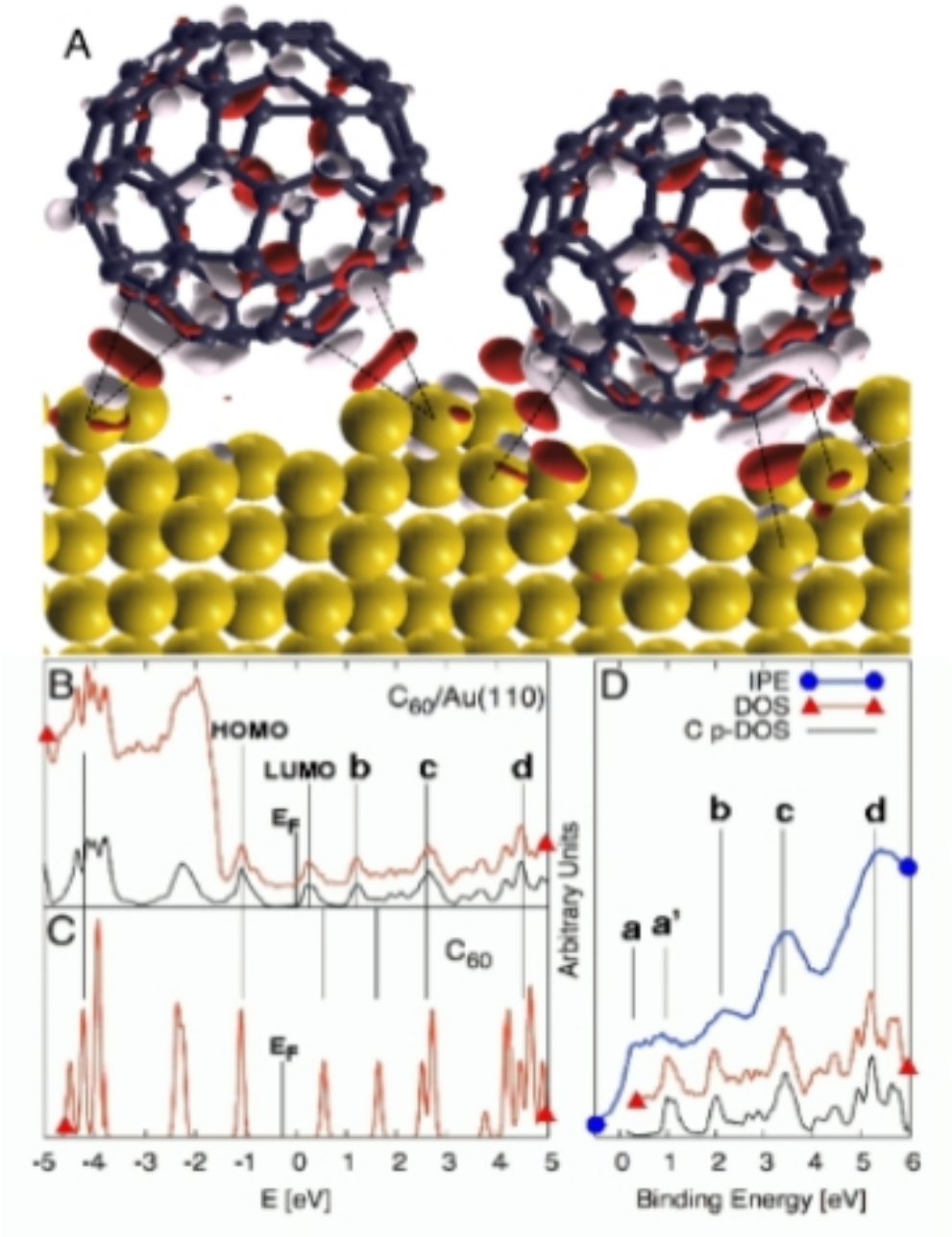


- Dye sensitized solar cell
- Squarainel + TiO2 + water
- Equilibration :
  20ps Car-Parrinello molecular dynamics

cp.x

R. Gebauer *et al*

Equilibrium structure and charge distribution



- Nano-structuration of substrate induced by absorption of organic molecules

C60 + Au surface

pw.x + pp.x

more applications at : www.quantum-espresso.org/samples.html
or at
www.quantum-espresso.org/wiki/index.php/Bibliography

EDUCATION

Quantum ESPRESSO with DEMOCRITOS, SISSA and ICTP are strongly involved in educational and dissemination activities related to material modelling from first principles.

past schools and tutorials:

http://www.quantum-espresso.org/wiki/index.php/Tutorials_and_Examples

-June 2010 workshop in Ireland

-July 2010 school at SISSA

-July 2010 CECAM tutorial at SISSA

-2011 School in Brazil

QE COMMUNITY

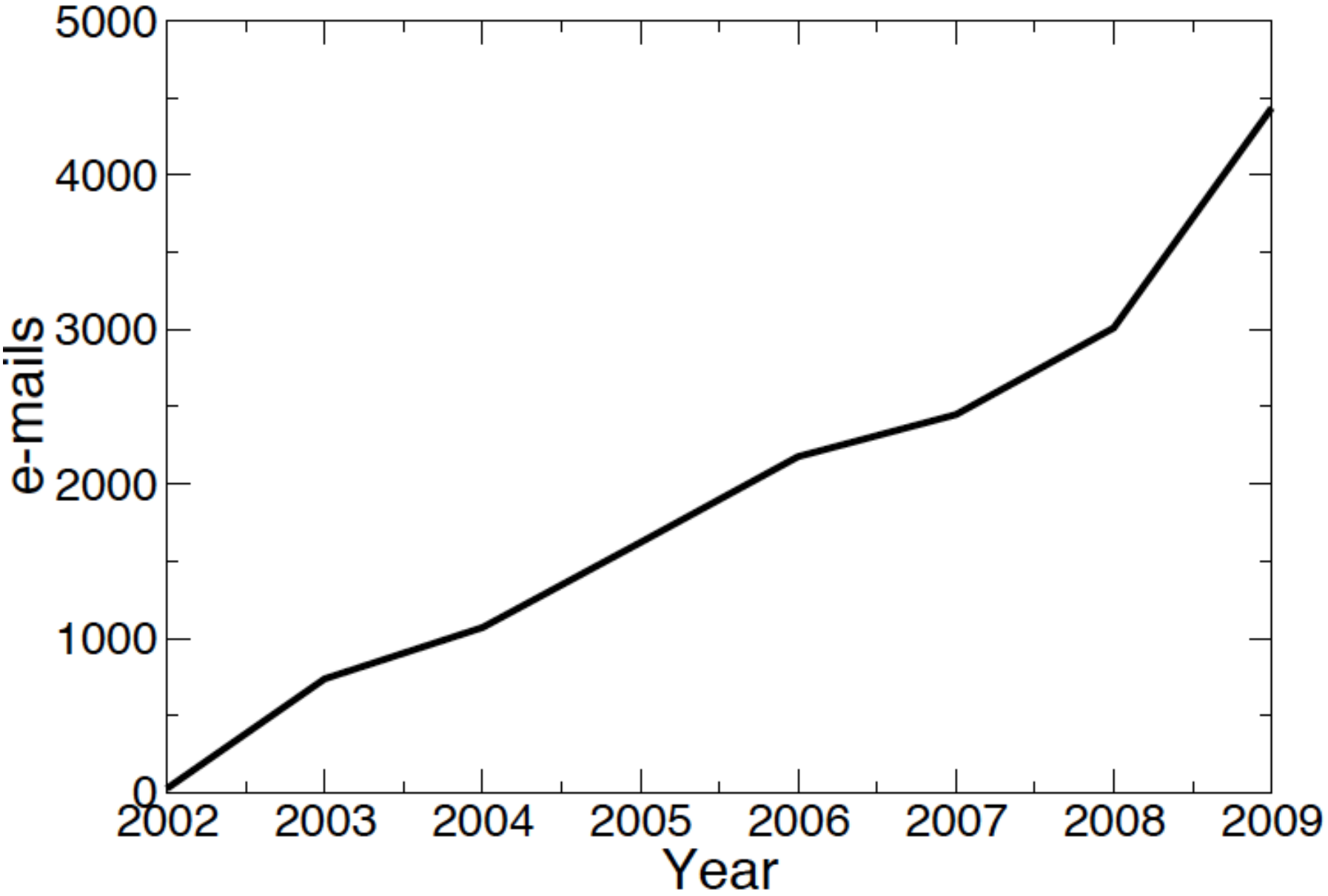
There is a vast open community behind us

- Users 1034 subscribers to the *forum*
- Developers 23, researchers with write access to the source code. Two ways for contributing:
  - Sending routines/changes to coordinators
  - Asking for write access on the cvs

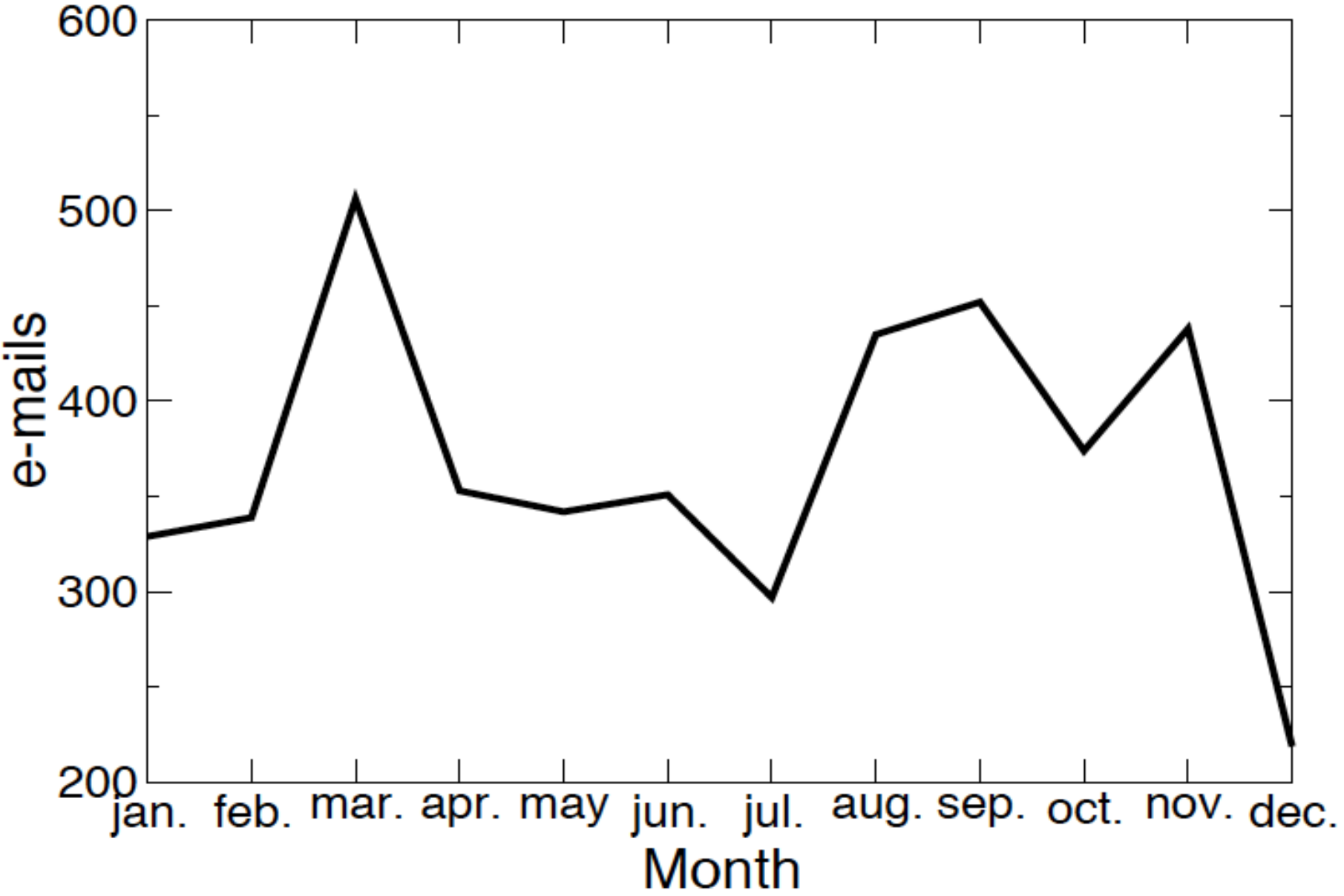
THE FORUM

pw_users@pwscf.org

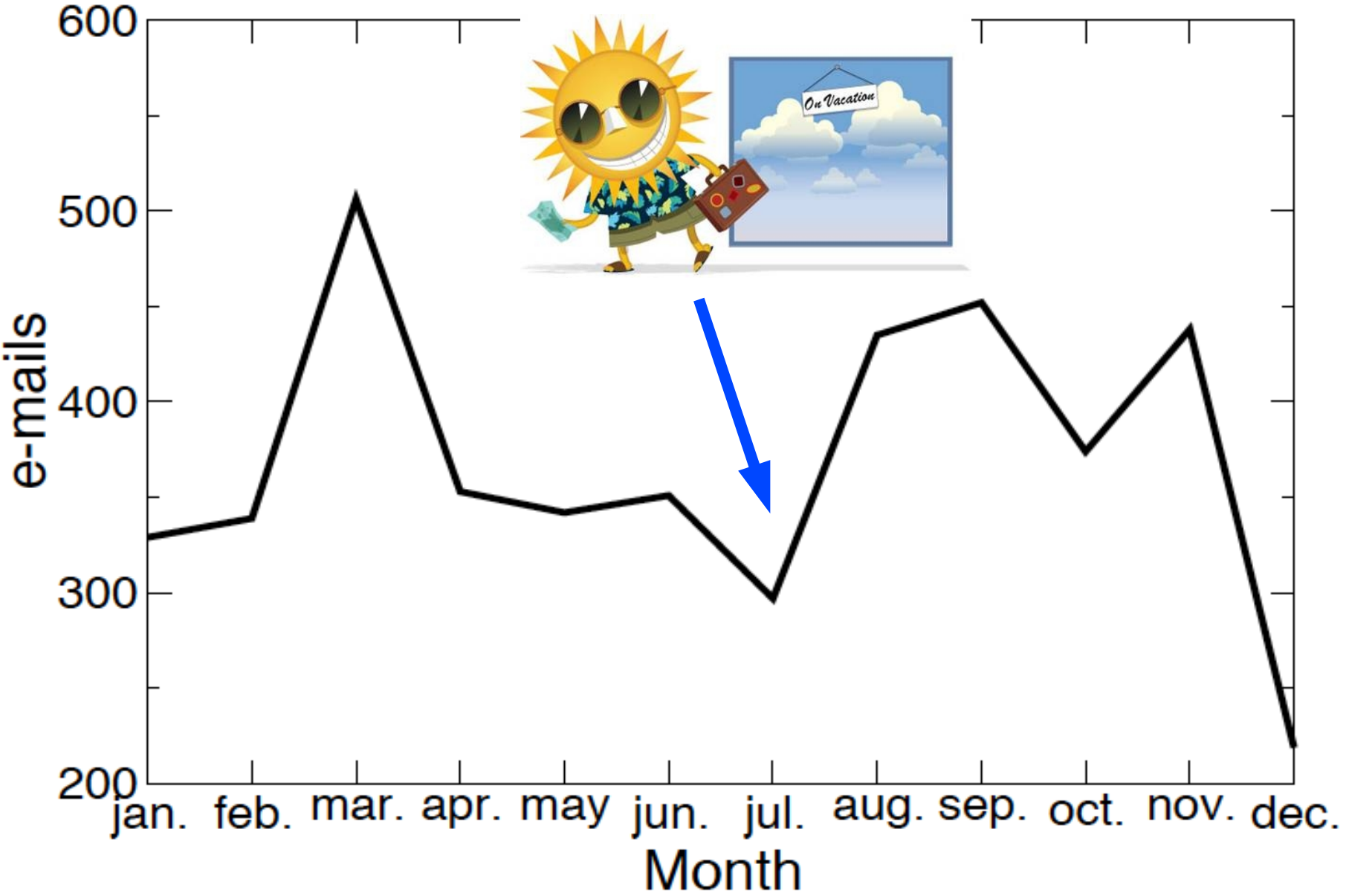
E-mails from the beginning of the forum



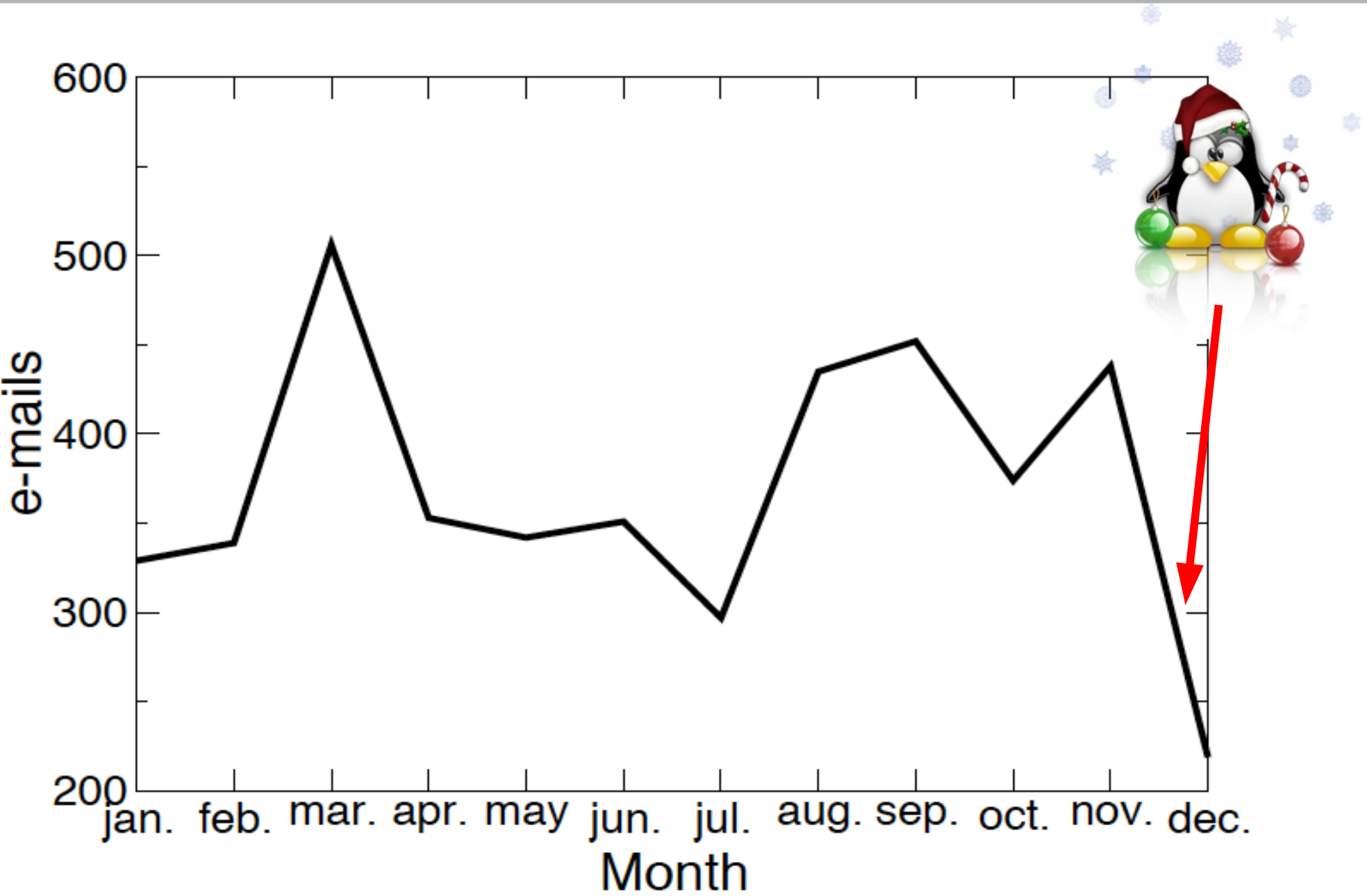
E-mails during 2009



E-mails during 2009



E-mails during 2009



THE QE-forge

QE-forge

- Mailing lists
- Forums
- Wiki
- Version management (cvs svn)
- Web pages
- Doc
- etc

What we expect to do

- Enhance the linux-like distribution character of QE, inviting more people to contribute.
- Explore the porting on of some parts on GPU (ICHEC, NVIDIA), GRID (e-lab).
- Improve QE-forge
- Improve exchanges with R&D.

THANK YOU