Centro di Competenza sul Calcolo Scientifico

Modellistica Chimica: Molecole nel Computer

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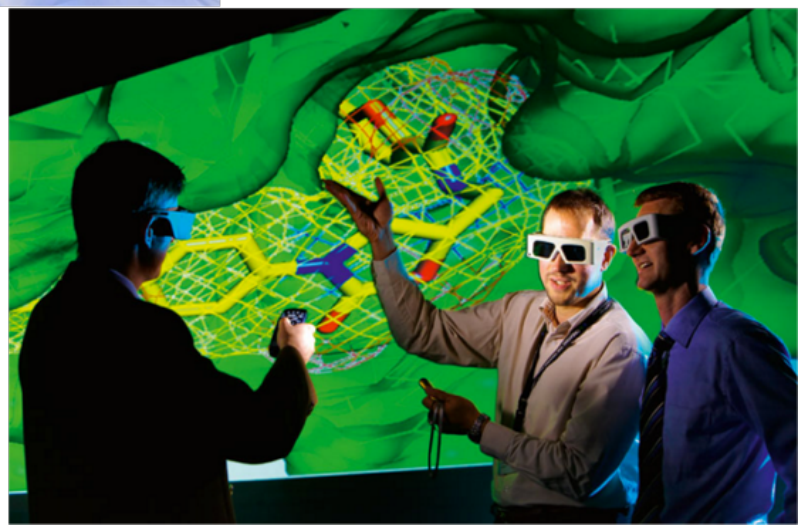
Modellistica Chimica: Molecole nel Computer

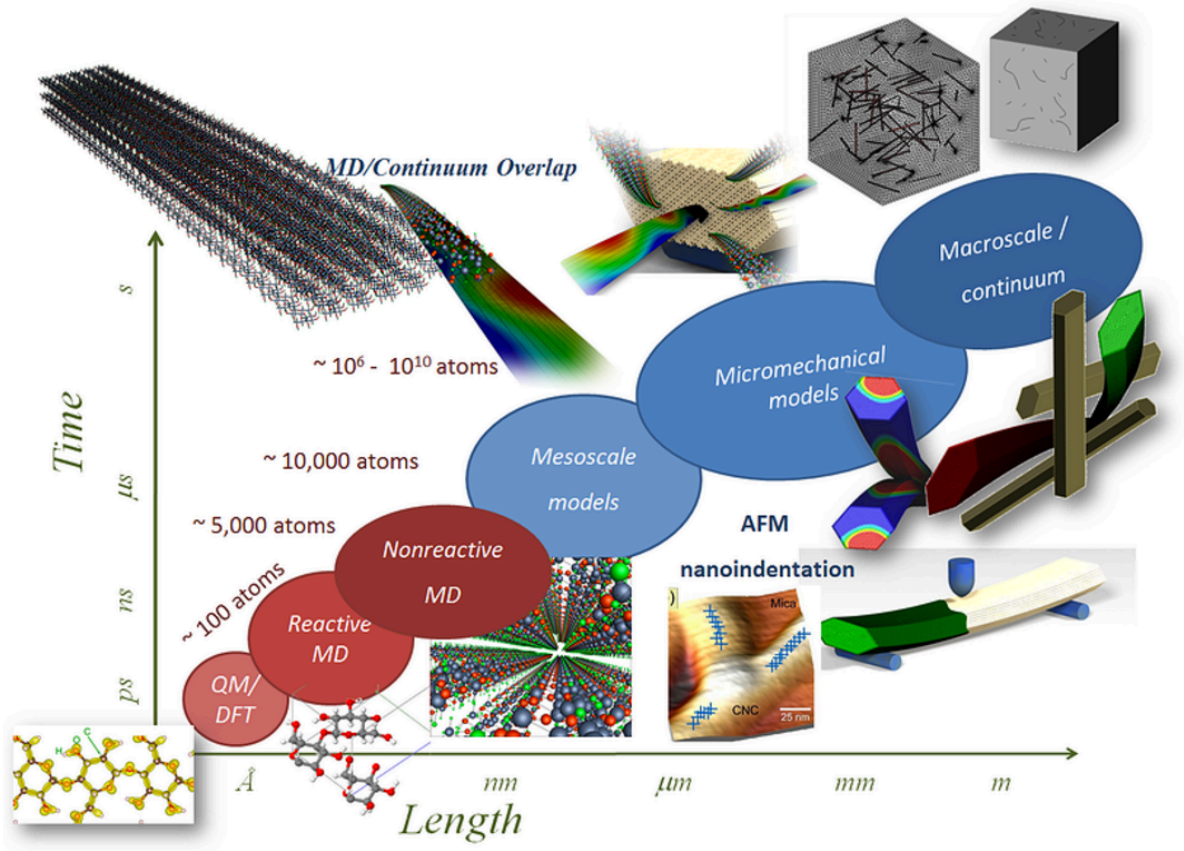
Teoria/
Modellizzazione

Esperimento



Modellistica Chimica: Molecole nel Computer

La modellizzazione in ambito chimico si rivolge ad un'ampia comunità scientifica che ha in comune una visione su scala atomistica della materia.



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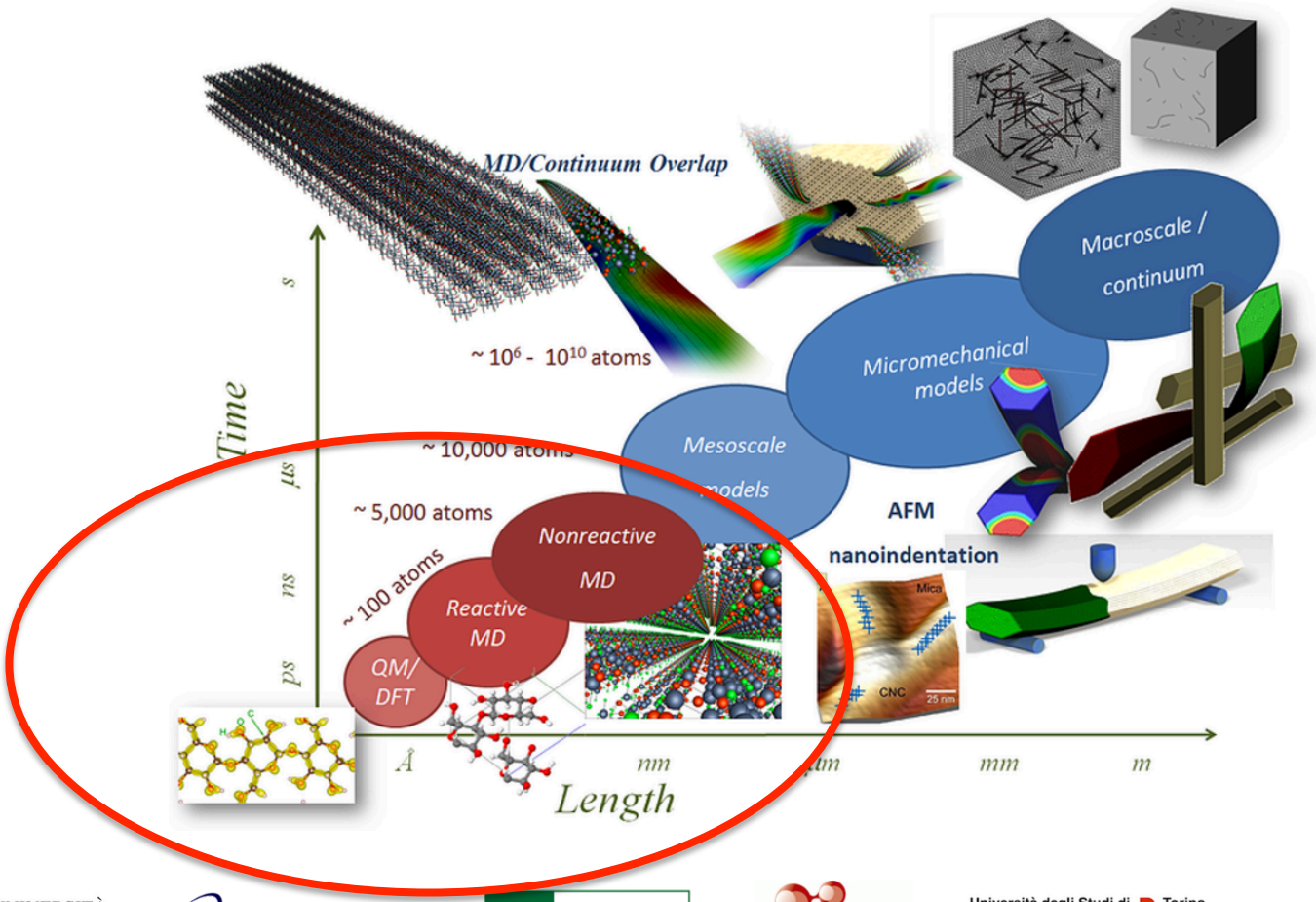
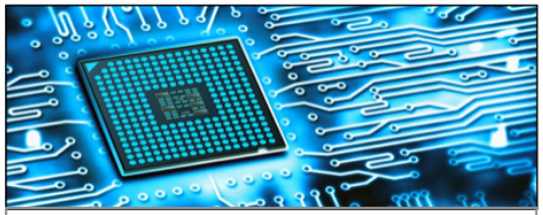
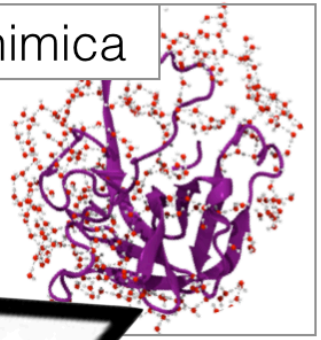
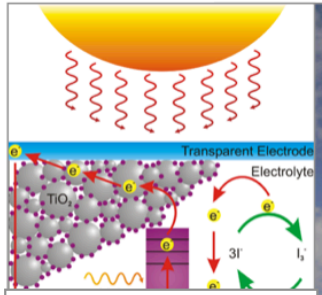


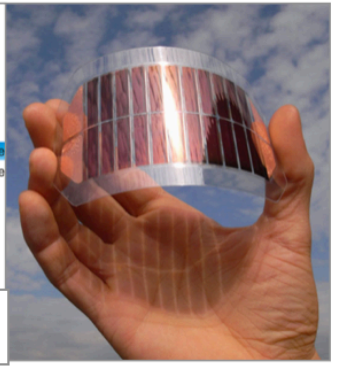


Materiali per l'elettronica

Biochimica

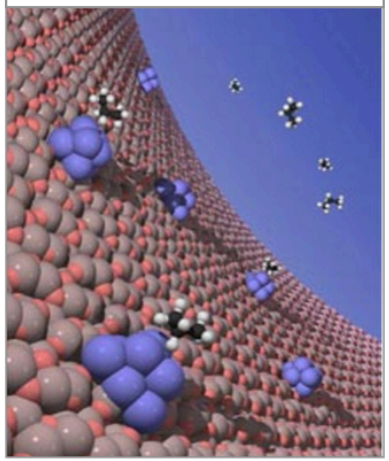




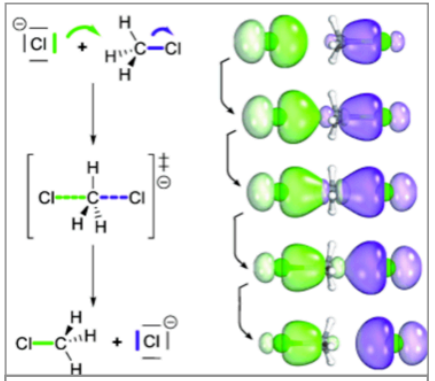


Celle solari

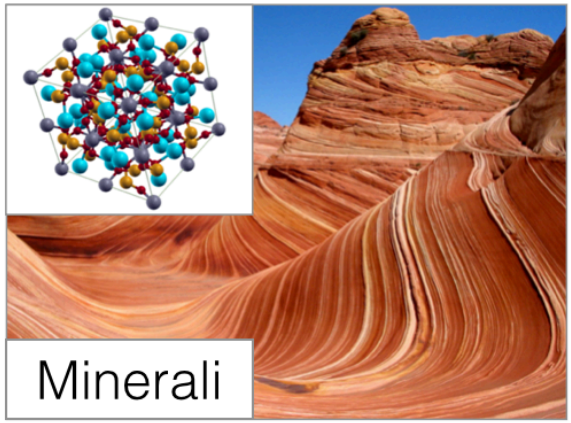
Superfici, catalisi



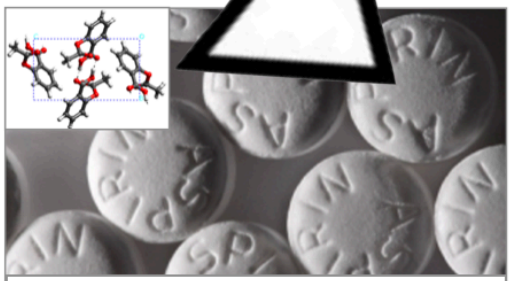
chimica



Reattività chimica

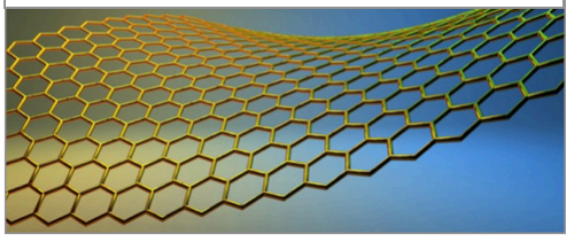


Minerali



Farmaci

Materiali Innovativi



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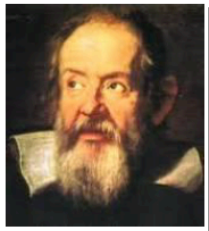
Modellistica Chimica: Molecole nel Computer

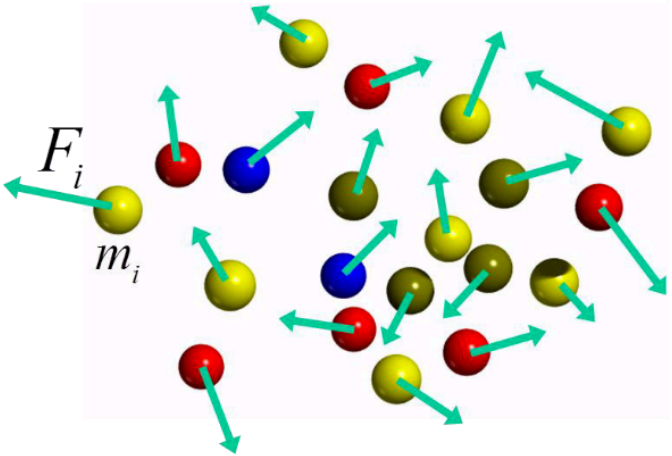
Esperimento



G Galilei

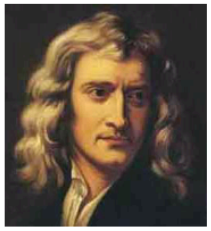
Osservare e misurare la posizione dei pianeti nello spazio e nel tempo

Teoria



$$V = V(x_1, \dots, x_{3N})$$

$$F_i = -\frac{\partial V}{\partial x_i} = m_i a_i \qquad i = 1, \dots, 3N$$



I Newton

Dalle forze di interazione (gravità) predire l'evoluzione spazio-temporale del sistema applicando **leggi fondamentali**

Modellistica Chimica: Molecole nel Computer

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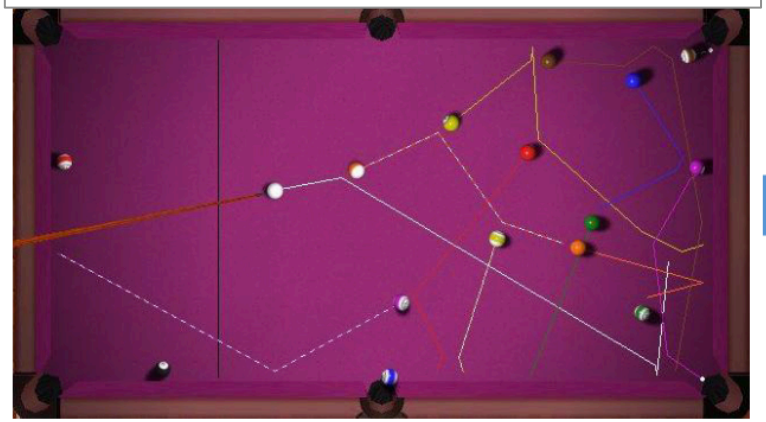
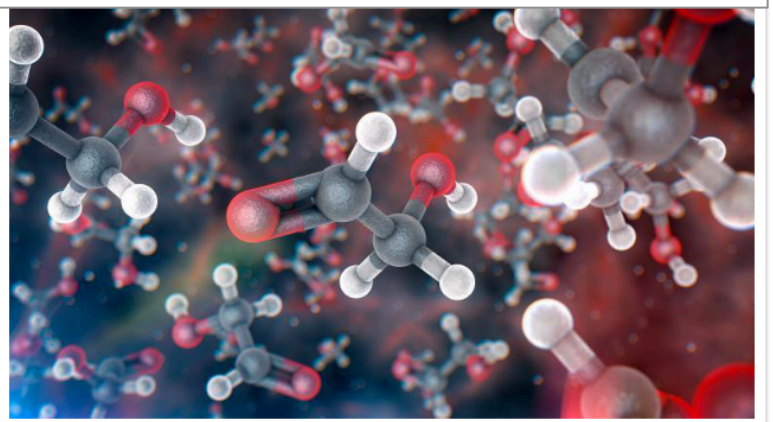
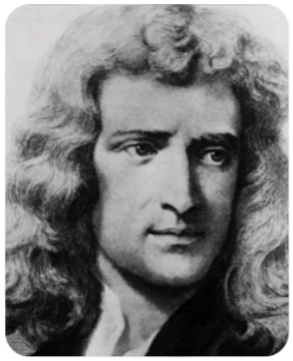
Scala Macroscopica



Scala Microscopica





I. Newton

$$F = m\,a$$

Meccanica classica

Traiettoria delle particelle

E. Schrödinger

$$\hat{H}\psi = E\psi$$

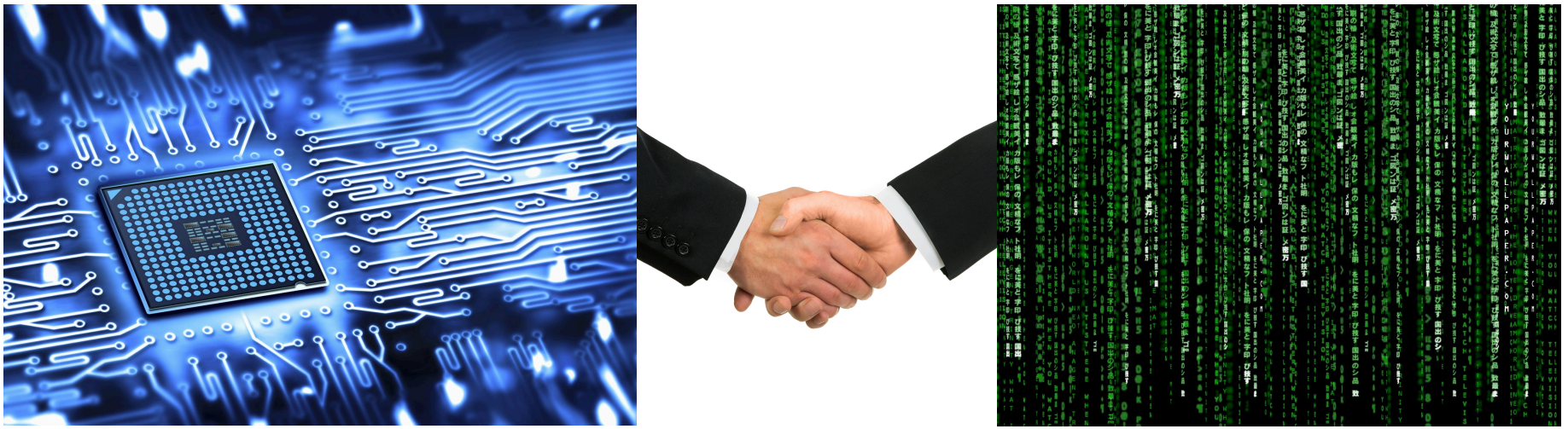
Meccanica quantistica

Funzione d'onda, probabilità

Modellistica Chimica: Molecole nel Computer

Hardware

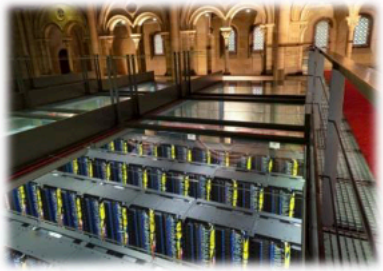
Software



HPC resources for computational chemistry

Gauss Centre Stuggart (CRAY XC40)

Cineca Bologna (Intel Phi)

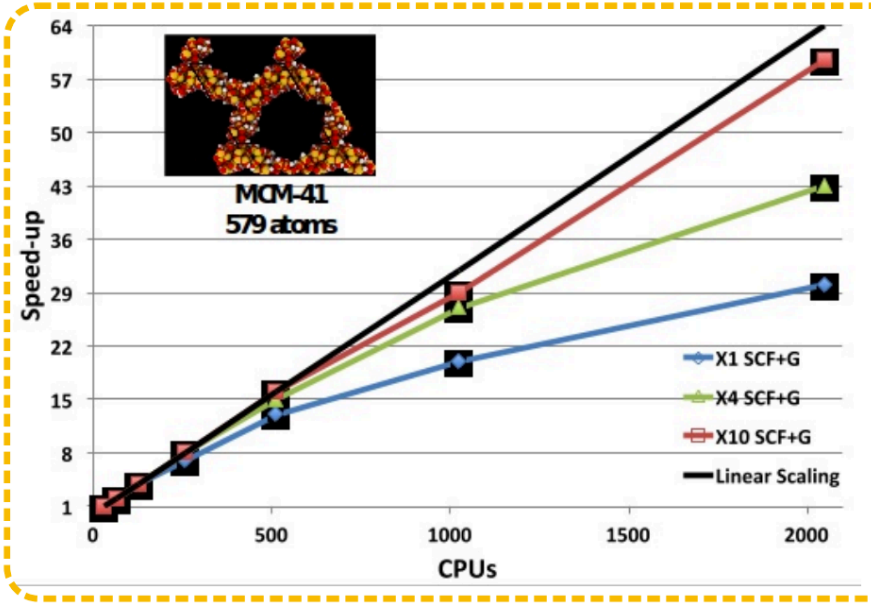


MN Barcelona (Intel Xeon)

Modellistica Chimica: Software

CRYSTAL

Sviluppato a Torino a partire dagli anni '70, oggi usato in tutto il mondo. Consta attualmente di 600 000 linee di codice (Fortran), ha eccellente scalabilità su macchine HPC.



CRYSTAL can be efficiently run both in parallel (P) and massive parallel (MPP) mode. The MPP mode is particularly suitable for studying large systems, drastically improving the speed-up and reducing the requirement for memory.

CRYSTAL solutions

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EDF
Saint-Gobain
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CRYSTAL 14

Crystal is a general-purpose program for the study of crystalline solids. The CRYSTAL program computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations.

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SUCCESS STORIES

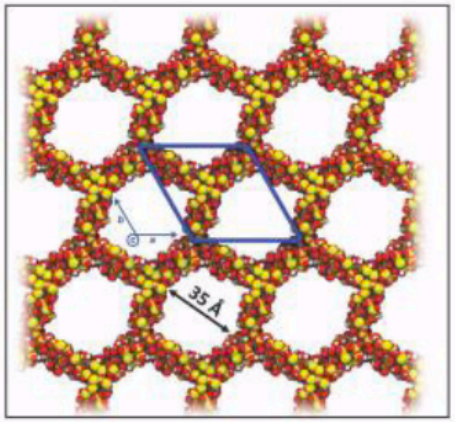
Harnessing European HPC to improve nanomedicines

Drugs can be delivered to specific areas of the body and benignly dispensed, using nanomedicines, and mesoporous silica is a material which possesses the properties to fulfil this role. To enhance its utility and answer fundamental scientific questions, Italian scientists have been analysing how biological agents interact with it at molecular level.

Nanomedicine offers exciting possibilities for medical practitioners to safely apply drugs without detrimental side effects. These are often caused when the human body's immune system reacts defensively to medicine, which it perceives as a threat. By deploying miniature couriers that 'smuggle' their payloads past the body's defences and even through cells walls, an array of potential new treatments could be introduced. To ensure the effectiveness of such treatments – and guarantee the welfare of patients – understanding the interactions between 'carrier' molecules, and the drugs they convey, is a prerequisite.

"Analysis has been undertaken to determine how the drug moves within the pores, and how easily it can be washed out the mesoporous silica by the body fluids"

"You can transport a drug by storing it in holes within certain materials," explains Professor Piero Ugliengo of the University of Torino. One of these is mesoporous silica – a substance containing evenly spaced periodic voids into which medicinal molecules can be inserted. Providing spaces of between two nanometres to fifty nanometres in diameter, this class of silica can help protect and deliver several types of drug, including ibuprofen. "Analysis has been undertaken to determine how the drug moves within the pores, and how easily it can be washed out the mesoporous silica by the body fluids," says Ugliengo. "Typically, these studies have been facilitated by experimental techniques like NMR (nuclear magnetic resonance spectroscopy), which help to illustrate the compound's mobility." Simultaneously biodegradable and biocompatible, silica's medicinal potential is widely recognised.



(Above) The MCM-41 mesoporous silica model. 579 atoms in 4.7x4.2x1.2 unit cell (drawn in blue).

However, little is known about the atomistic mechanisms that actually hold drugs in place within these minute, silica cages. "The walls of these molecular vessels are rather complicated. They're basically amorphous," explains Ugliengo. "A number of active sites, called silanol groups, exist on their surface at molecular level. Chemically, these help to form a hydrogen bond between the silica and the 'passenger' molecules that are the active clinical agents. This is basic chemistry, and fairly straightforward. But an important aspect of this relationship, and a

Project title: Mesoporous silica for drug delivery: a quantum mechanical simulation
Project leader: Prof. Piero Ugliengo, Associate Professor at the Università di Torino
Project details: This project was awarded 20,000,000 core hours on SuperMUC @ GCS@LRZ

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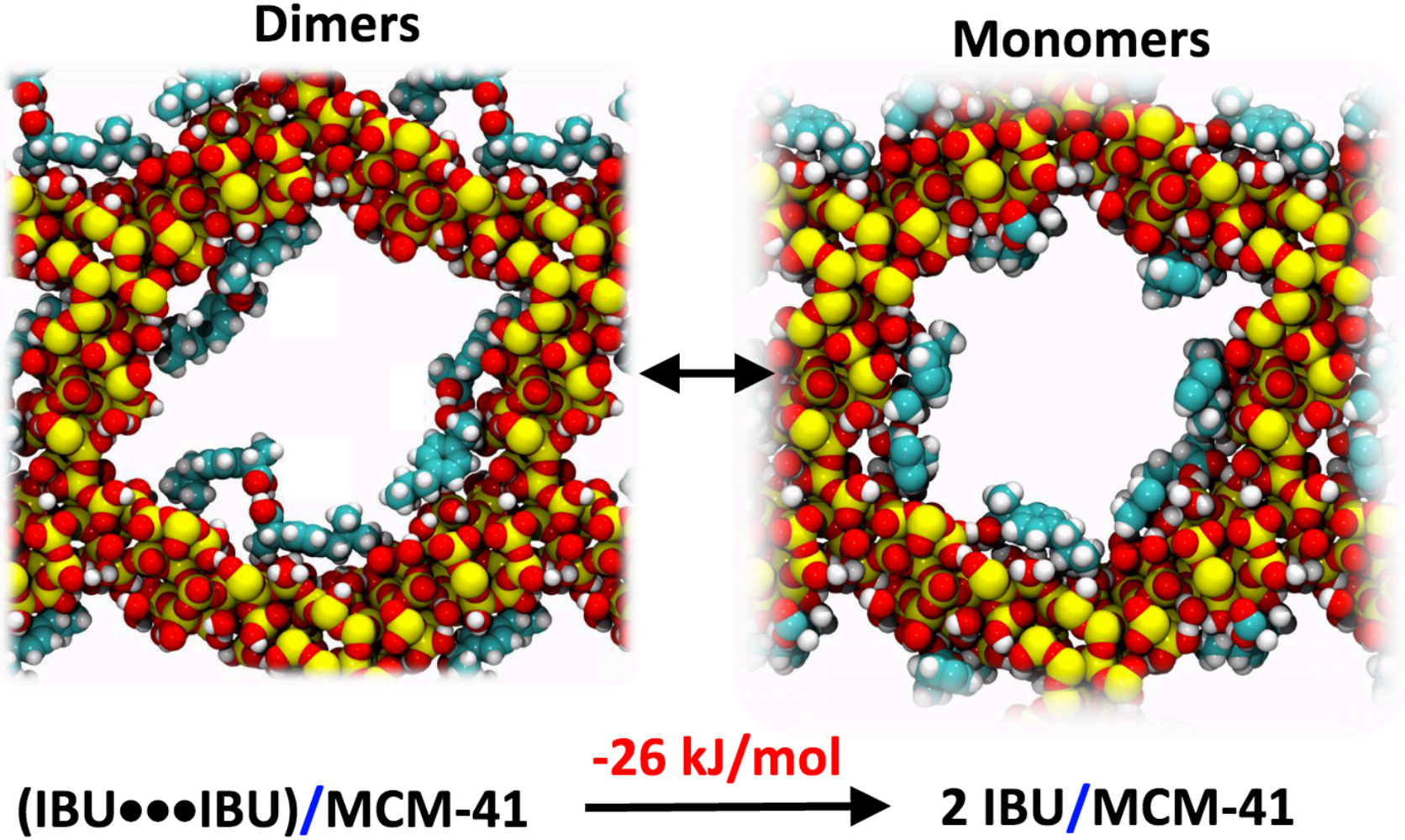

Modellistica Chimica: Il Centro Interdipartimentale NIS

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This is the new NIS website. The old site can be still reached here.

News and Highlights

Job Day Unito, 26th October 2016 Students of the University of Torino meet representatives from the most important Italian and international industries More

Nis Colloquium, 6th-7th October 2016 "Harnessing the Power of Light

Nanostructured Interfaces and Surfaces

Inter-departmental centre

NIS is an Inter-departmental research Centre bringing together more than 180 researchers from 5 Departments of the University of Torino:

- Chemistry
- Physics
- Drug Science and Technology
- Life Sciences
- Earth Sciences

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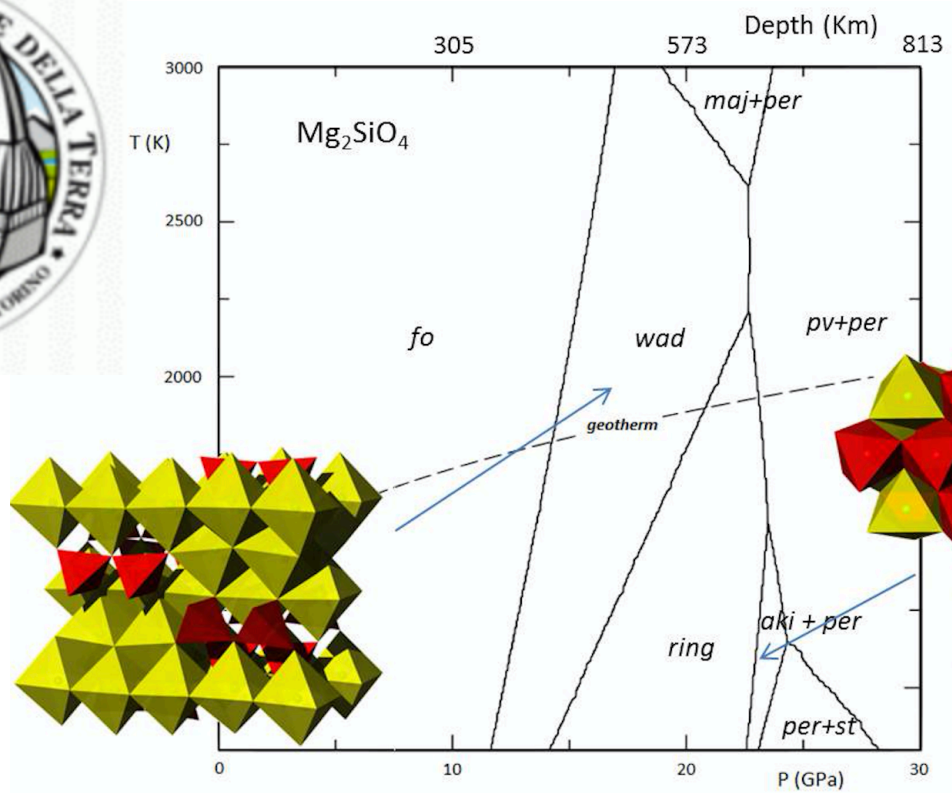
Modellistica Chimica: Diagrammi di Fase dei Minerali



fo: forsterite
wad: wadsleyite
ring: ringwoodite
maj: majorite
pv: perovskite
per: periclase
aki: akimotoite
st: stishovite

Wadsleyite: Mg_2SiO_4
Space group *Imma*

Akimotoite: $MgSiO_3$ with *ilmenite* type structure. Space group $R\bar{3}$

$SiMg_2O_4 \rightarrow MgSiO_3 + MgO$
(*ring*) (*aki*) (*per*)

Ringwoodite: *spinel* type structure

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Grazie per l'attenzione!

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