



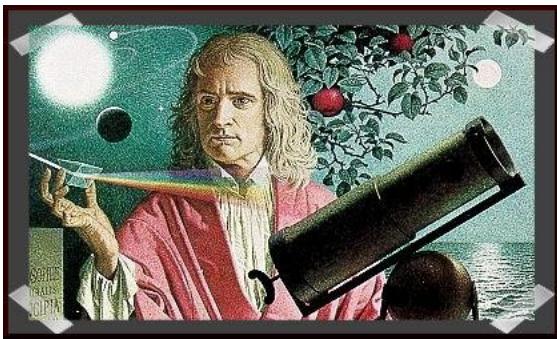
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Research activity in Computational Chemistry @DSCG

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Computational Chemistry

Computational chemistry is the branch of theoretical chemistry that deals with the development of mathematical models, based on classical mechanics and quantum mechanics, capable of simulating chemical systems, in order to calculate the physical characteristics and predict chemical properties.



Newton's Equations (1687)

$$\frac{\partial^2 \mathbf{r}_i}{\partial t^2} = \frac{\mathbf{F}_i}{m_i} = -\frac{\nabla_i U(\mathbf{r})}{m_i}$$

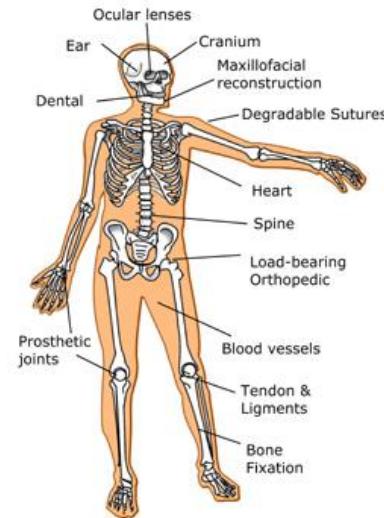
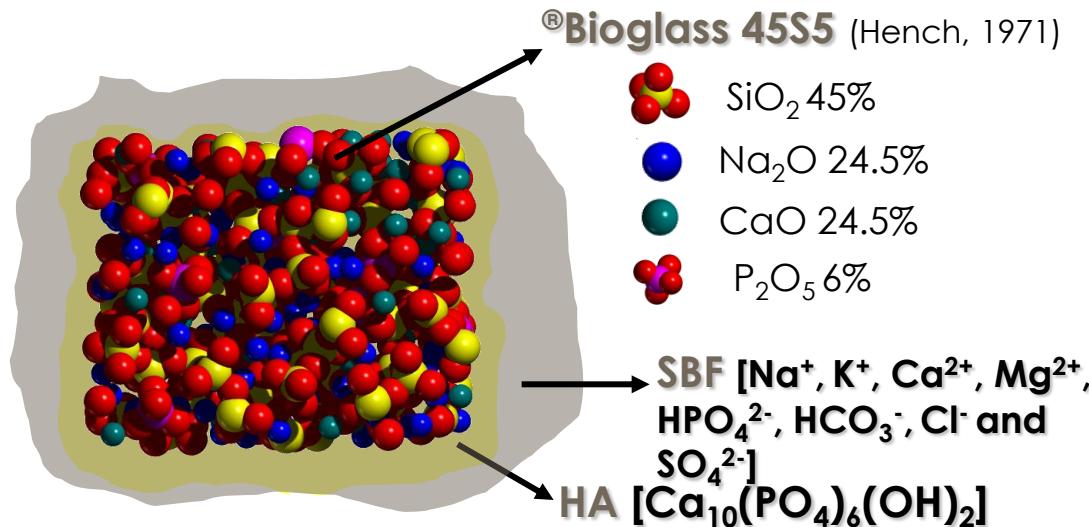


Schrödinger Equation (1927)

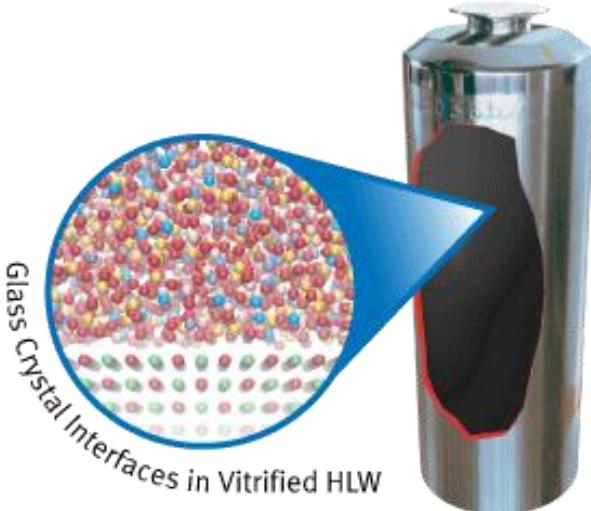
$$-\frac{\hbar}{i} \frac{\partial}{\partial t} \Psi(r, t) = H\Psi(r, t)$$

Silica Based Glasses

Orthopedic and Dental implants:



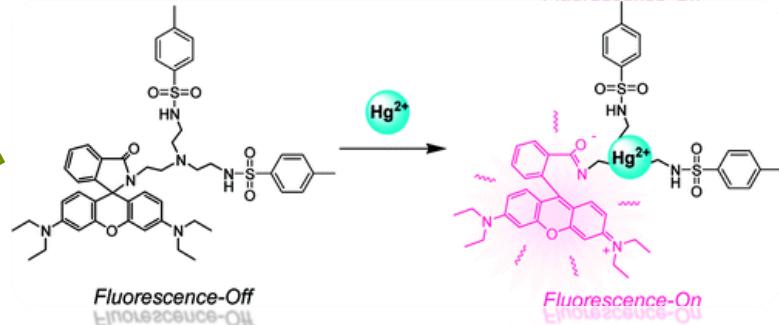
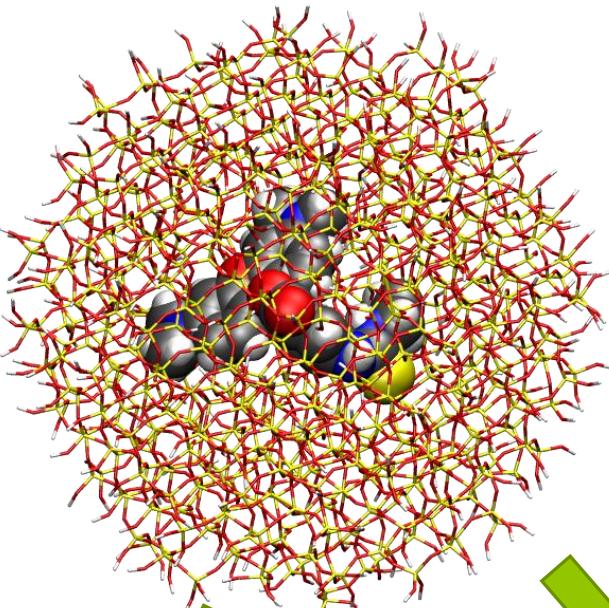
Nuclear waste confinement



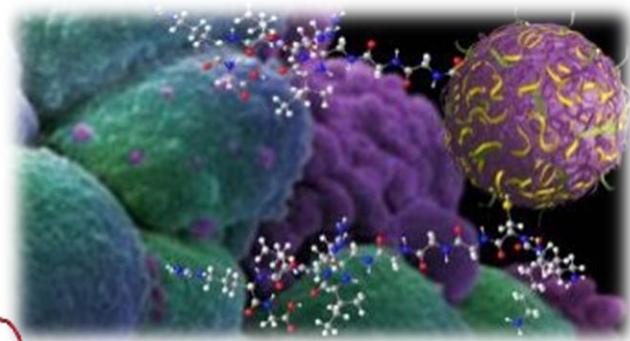
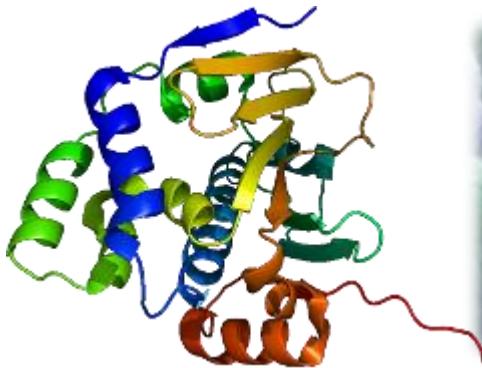
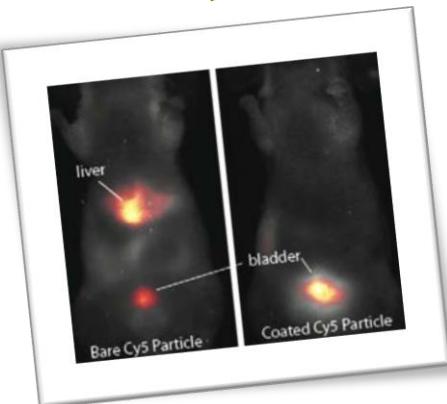
Atomic Energy and Alternative Energies
Commission - France



Fluorescent Nanoparticles



CHEMOSENSORS



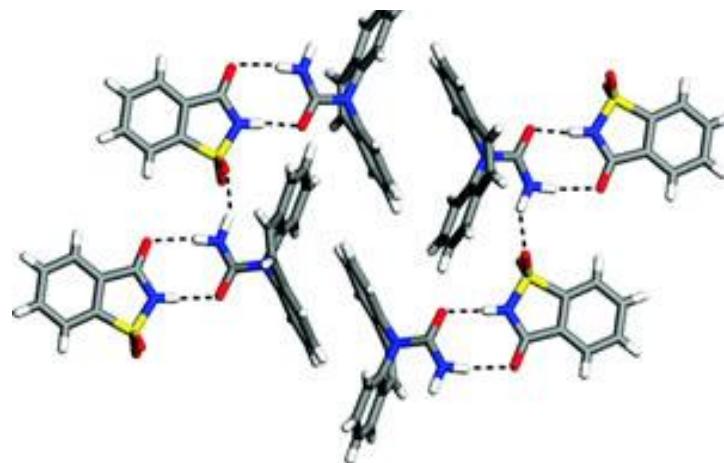
Drug delivery systems

Bright labels in nanomedicine
(imaging & diagnostics)

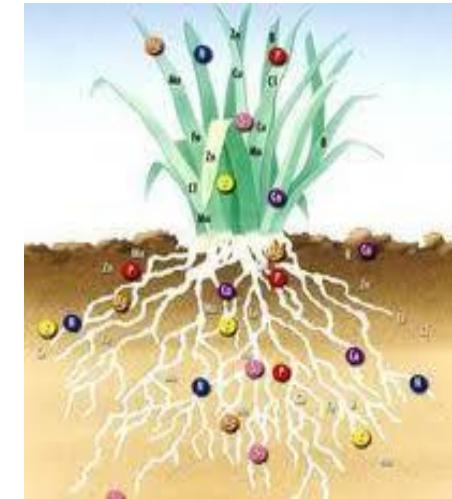
Pigments



Drugs



Crystal Polymorphism



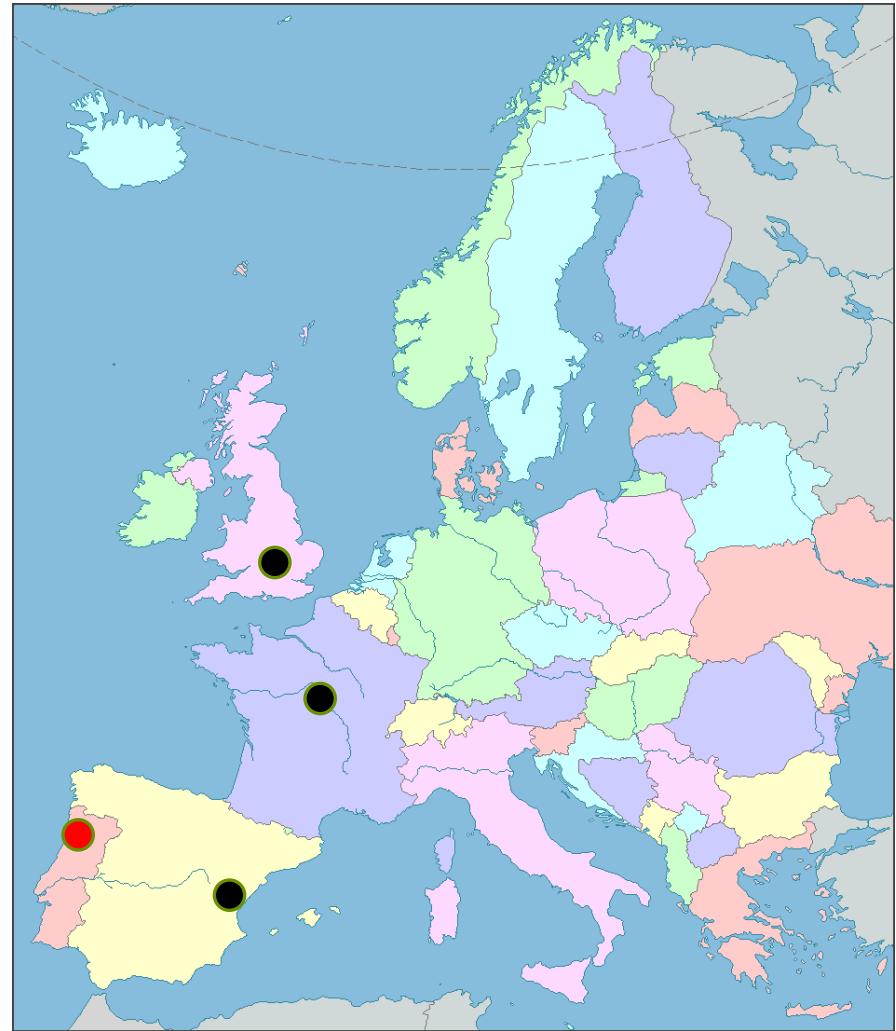
Agrochemicals

The different phases of crystalline or amorphous, while containing the same active molecule may have chemical, physical and mechanical properties that are very different, with substantial consequences on their use, handling and absorption.

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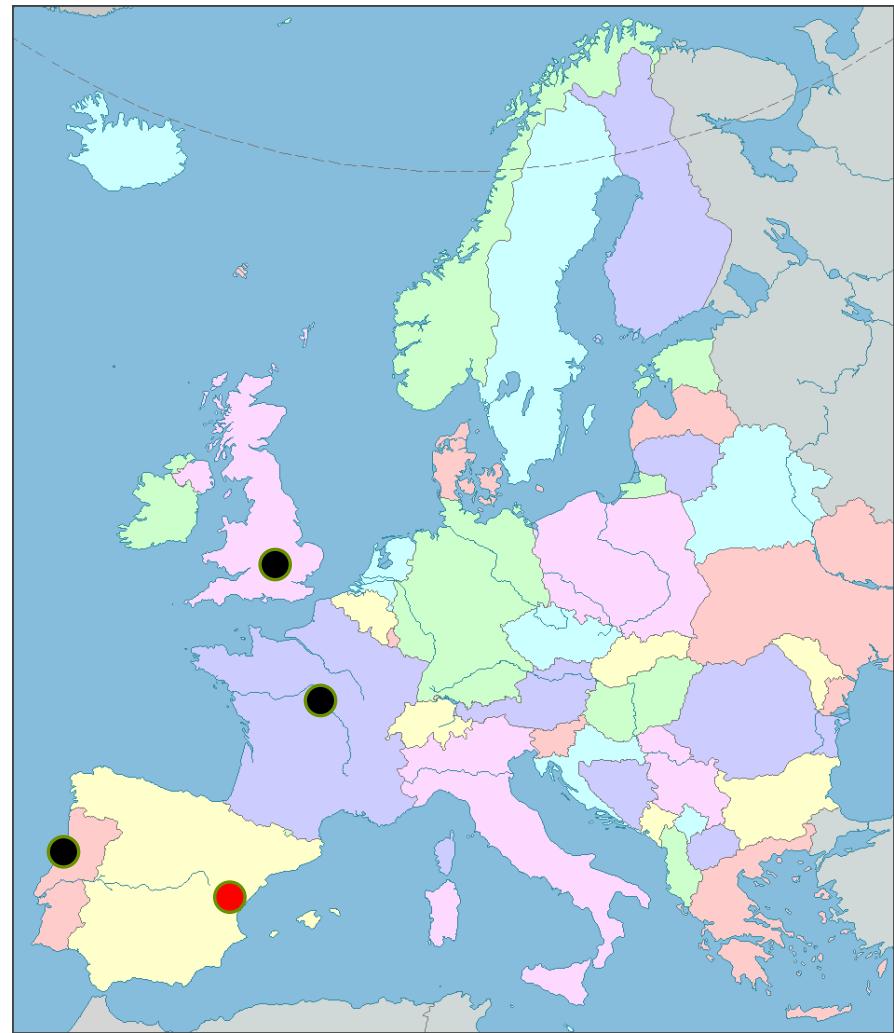
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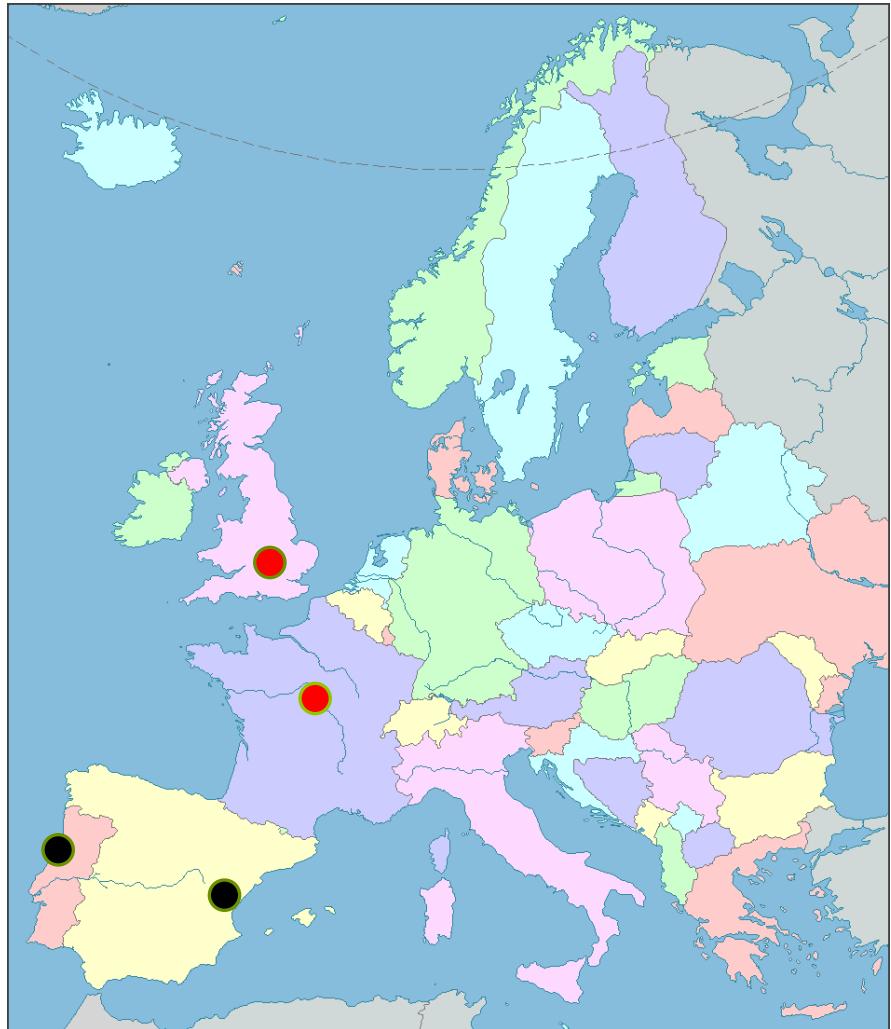
Collaborations



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Collaborations

