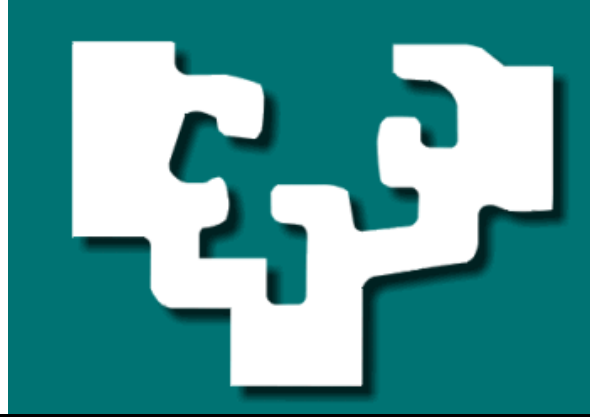


Eman ta zabal zazu

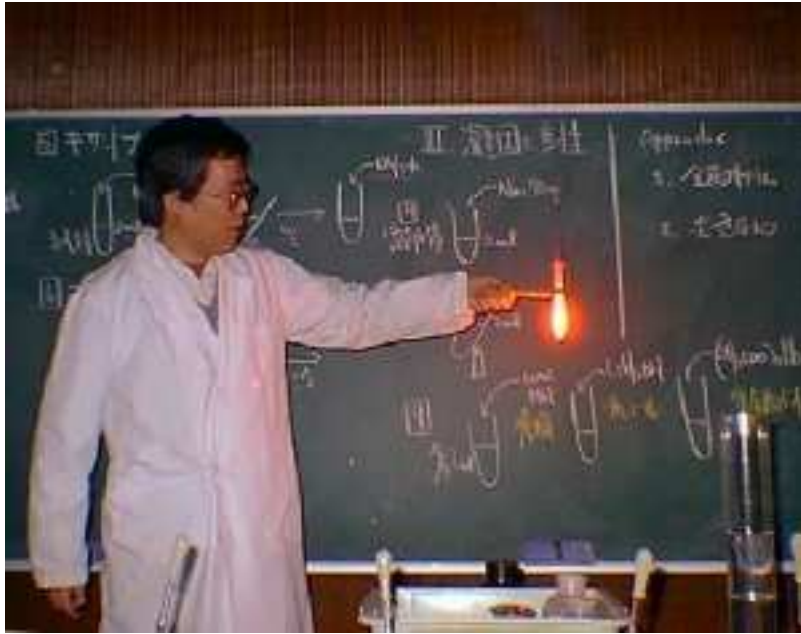


Cálculo Intensivo en Investigaciones  
Físico–Químicas.

**J. M. Ugalde**

Kimika Fakultatea, Euskal Herriko Unibertsitatea, P.K. 1072,  
20080 Donostia, Euskadi (Spain)

**<http://www.sc.ehu.es/chemistry/theory>**



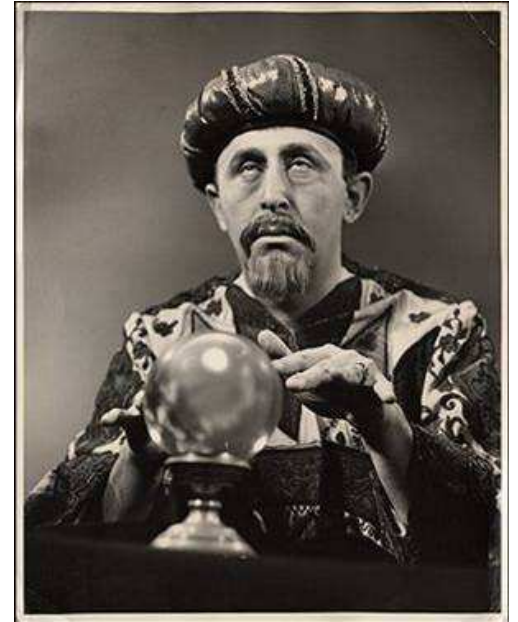
La química es la transformación de la materia.

# Químicos trabajando

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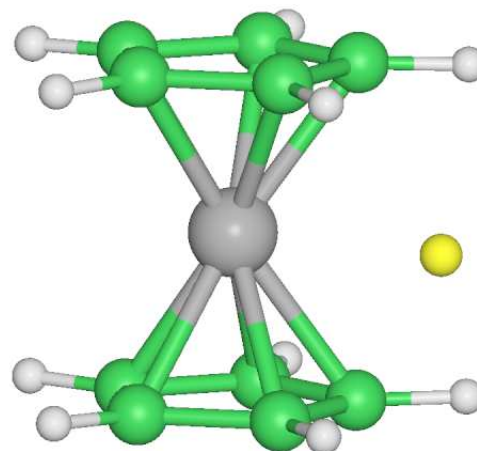
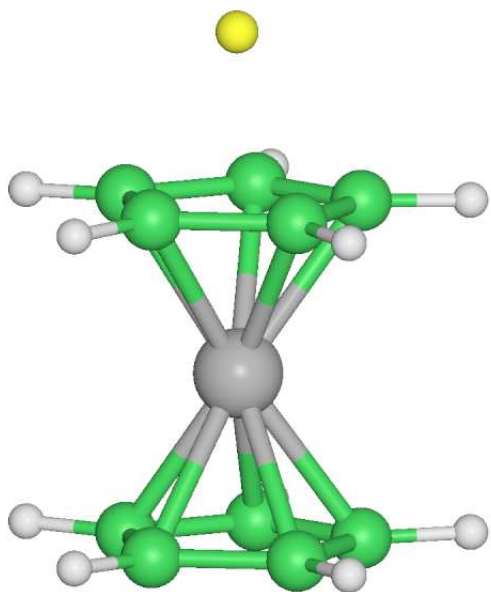
Sin embargo, hoy en día ...  
Podemos predecir que materiales son posibles y cuales son sus propiedades.



# Predicción

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A. Irigoras, I. Silanes, J. M. Mercero, J. M. Ugalde  
**The Ferrocen–Lithium Cation Complex in the Gas Phase**  
*J. Am. Chem. Soc.*, **123** (2001), 5040



# Verificación



Matthias Wagner, et al.

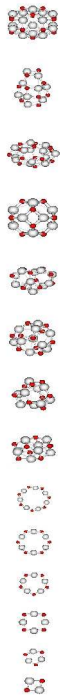
*"[1.1]Diborataferrocenophane:  
A Highly Efficient Li<sup>+</sup>  
Scavenger."*

Angew. Chem. Int. Ed., **42**  
(2003) 924.

"As predicted by Ugalde et al.  
the Li<sup>+</sup>-ferrocene ... is a novel  
type of redox-switchable  
lithium scavenger"

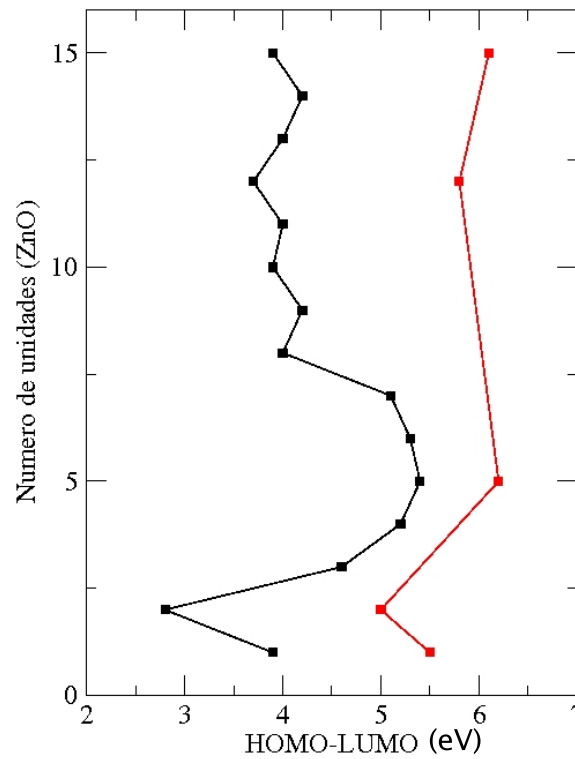
# Crecimiento de Nanocristales: Nanotecnología

## Predicción

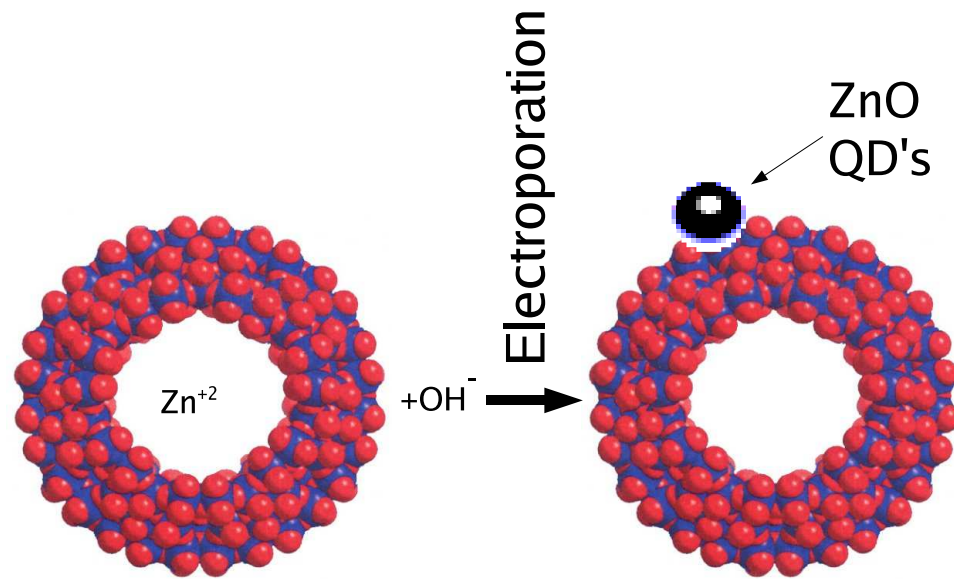


J. M. Matxain et al.  
J. Am. Chem. Soc. **125**, 9494 (2003)

## Verificación



Z. A. Schelly et al.  
Nanotechnology, **17**, 4713 (2006)



Z. A. Schelly *et. al.*

**Synthesis and Bandgap Oscillations of uncapped ZnO clusters by electroporation of vesicles**

*Nanotechnology*, **17** (2006) 4713



## 2e-3D-QS's: Nanotechnology.

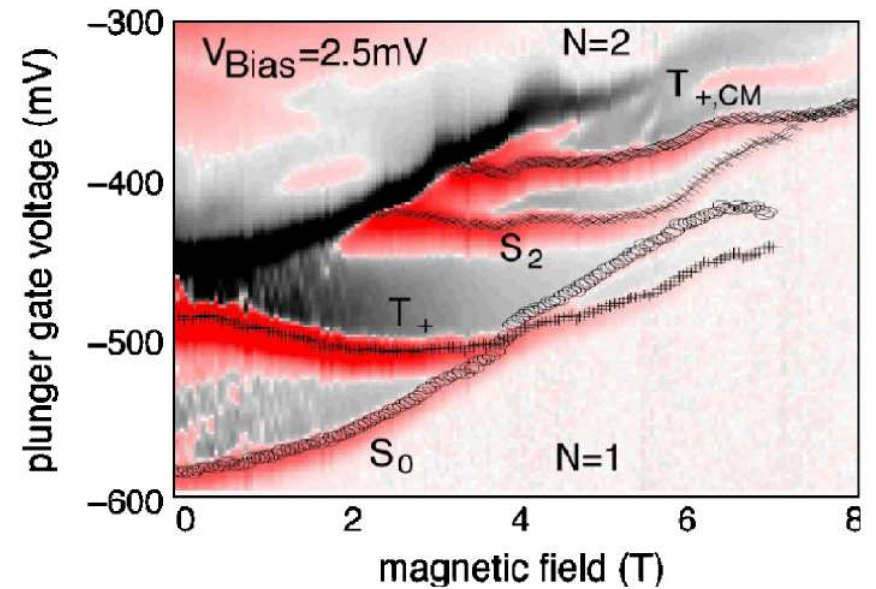
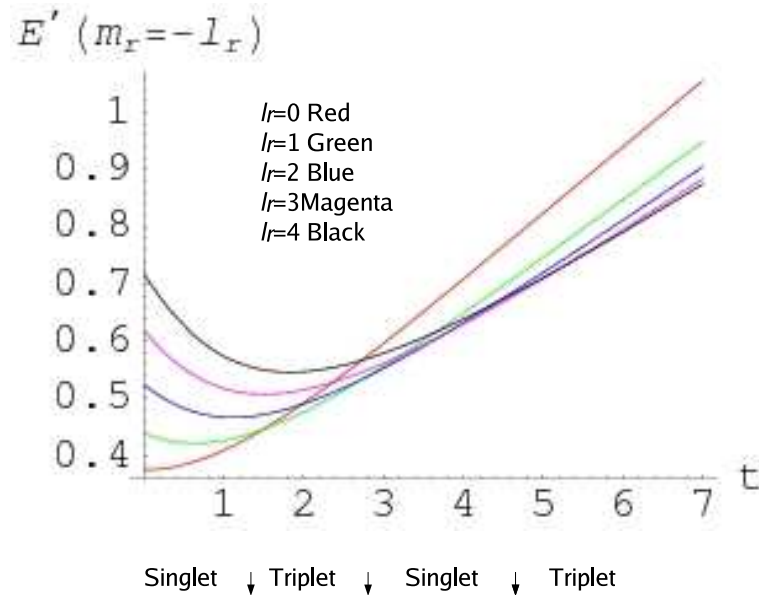


- Quantum dots (QDs), nano-sized semiconductor crystals that, when stimulated by laser light, can fluoresce in a rainbow of colors. QD's can be attached to peptides or antibodies that recognize specific cancer cells, and then using the dots to isolate individual cancerous areas.

C. Seydel, *Science*, **300**, 80 (2003).

## Predicción: Spin-flipping

## Verificación (!)



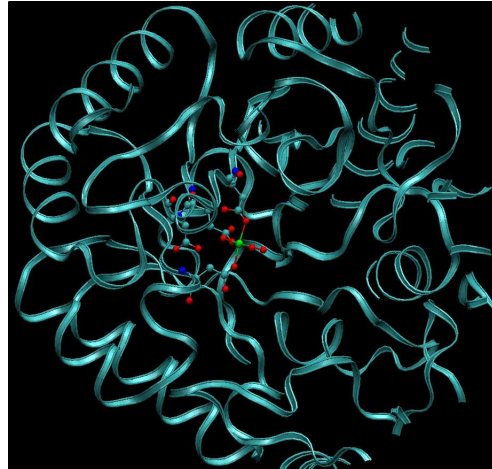
X. Lopez, J. M. Ugalde, L. Echevarría, E. V. Ludeña  
*Phys. Rev. A.*, **74**, 042504 (2006)

C. Ellenberger *et al.*  
*Phys. Rev. Lett.* **96**, 126806 (2006)

# Predicción

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El "bonding-site" del  $\text{Al}^{+3}$  en entornos proteicos:



E. Rezabal, J. M. Mercero, X. Lopez, J. M. Ugalde

**The coordination shells of Al(III) and Mg(II) in model protein environments. Which protein ligands facilitate Mg/Al exchange ?**

*Journal of Inorganic Biochemistry.* **100**, 374 (2006)

# Verificación

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Estamos esperando ...



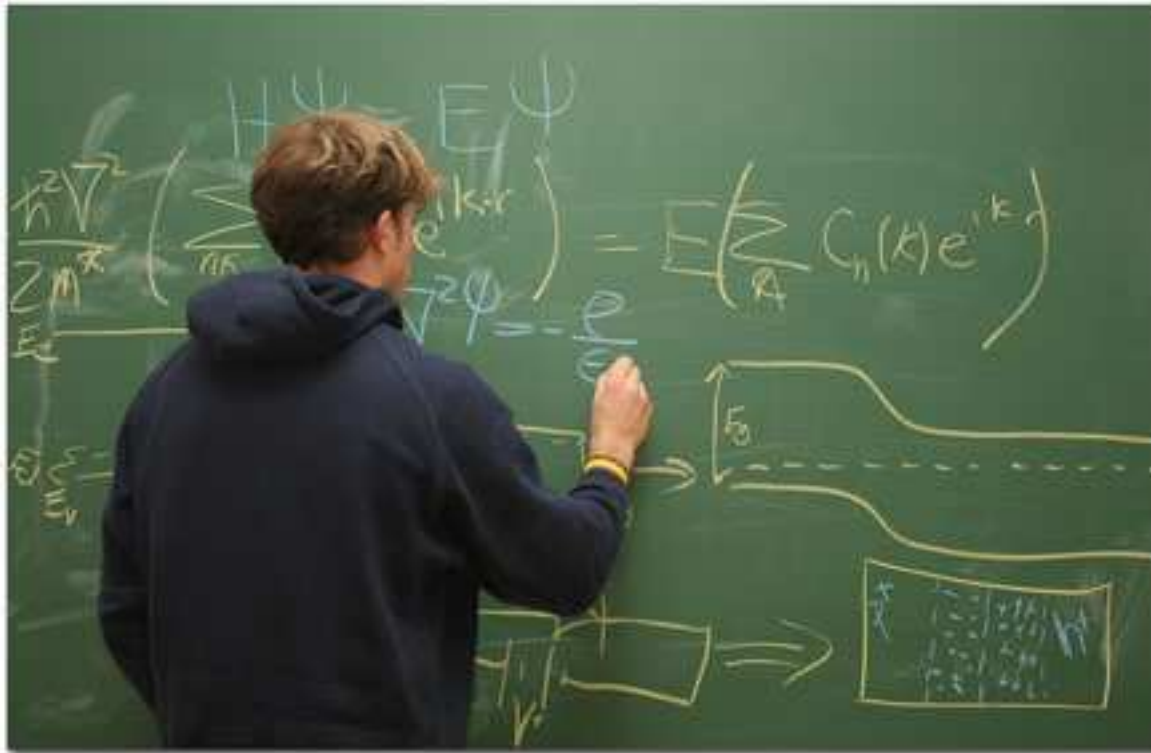
con impaciencia !!.

# Ecuación de Schrodinger

$$H\Psi = E\Psi$$




# Interpretación



# Red de Datos



- Paralelismo másivo
- Transferencia de datos entre CPU's
- Red:
  - Rápida
  - Estable
  - Segura

**i2BASK**