



**UNIVERSIDAD
NACIONAL
DE LA PLATA**

I F L P



CONICET
U N L P

Aplicación de la Mecánica Cuántica para el estudio de Materiales

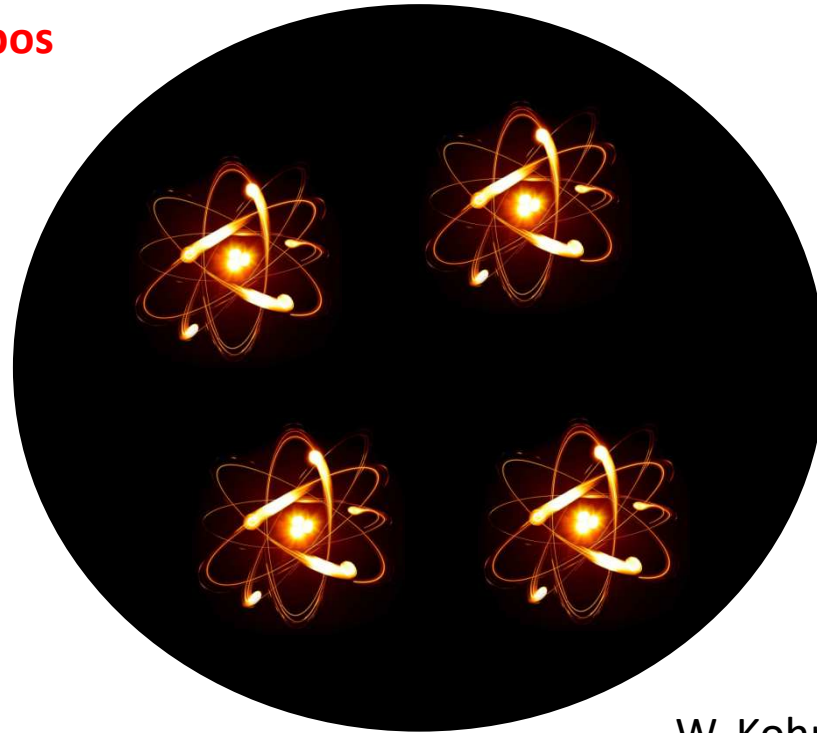
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Sistema de muchos cuerpos



Ecuación de Schrödinger

E. Schrödinger (Nobel de Física 1933)

Ecuación de Kohn-Sham

W. Kohn (Nobel de Química 1998)



Describe al sistema como tal.



No existe solución exacta.



Determinación de la función de onda.



Observables dependen de la función de onda.



Evolución con el tiempo, estados excitados.



Dinámica.

Teoría de la Funcional Densidad



Aproximación del sistema.



Solución aproximada.



No interesa la función de onda, si la densidad.



Observables dependen de la densidad.



Evolución con el tiempo, estados excitados.



Dinámica.

Qué se puede estudiar?

- **Propiedades estructurales**

Determinación de estructuras cristalinas, optimización de posiciones atómicas en moléculas y superficies. Comparación con: Rayos X, XANES, EXAF, IR, RAMAN

- **Propiedades magnéticas e hiperfinas.**

Magnetización total y por átomo, estudio de diferentes configuraciones magnéticas, propiedades hiperfinas. Comparación con medidas de magnetización VSM, SQUID, Difracción de Neutrones, espectroscopia Mössbauer, PAC, NMR, NQR, EPR.

- **Propiedades Ópticas,** comparación con espectros de absorción, UV-vis.

- **Adsorción de moléculas en superficies,** comparación con STM, AFM, TPD.

- Etc.

Limitaciones

- Efectos de temperatura.  Ab-initio Molecular Dynamics (AIMD)

- Recursos computacionales.

Cuando el experimento complementa a la teoría.

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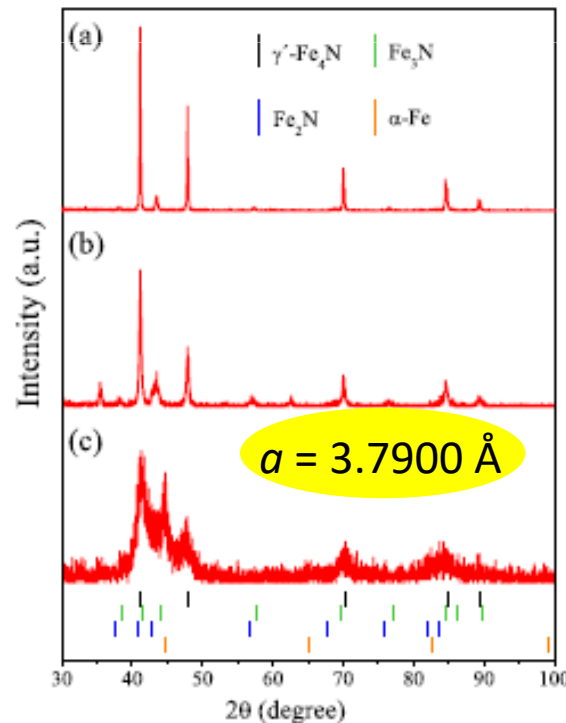
First principles and experimental studies of the structural and magnetic ground state of the ternary compound MnFe_3N



A.V. Gil Rebaza ^{a, b, *}, A.M. Mudarra Navarro ^a, J. Martinez ^{a, c}, E.L. Peltzer y Blancá ^b

DFT

- Estructura cristalina: $P4/mmm$
- Parámetro de red: 3.7903 \AA
- Ordenamiento antiparalelo entre los átomos de Mn y Fe, con momento total $4.75 \mu_B$.



Experimento

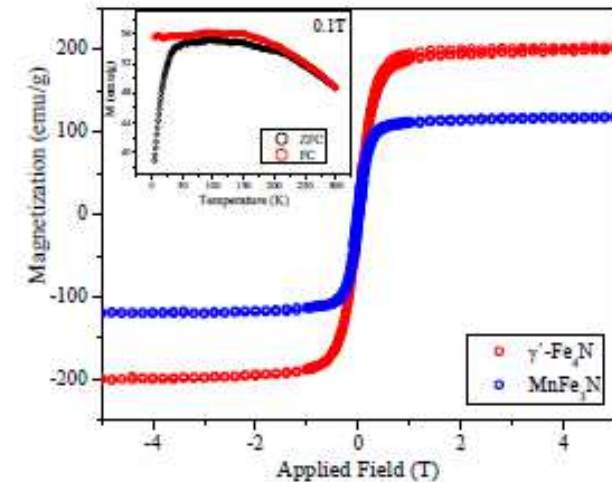


Fig. 7. Magnetization curve for the $\gamma\text{-Fe}_4\text{N}$ and MnFe_3N at 5 K.

$M_T = 5.03 \mu_B$

Synthesis, Crystal and Magnetic Structure of the Double Perovskites A_2NiMoO_6 (A = Sr, Ba): A Neutron Diffraction Study

Experimento

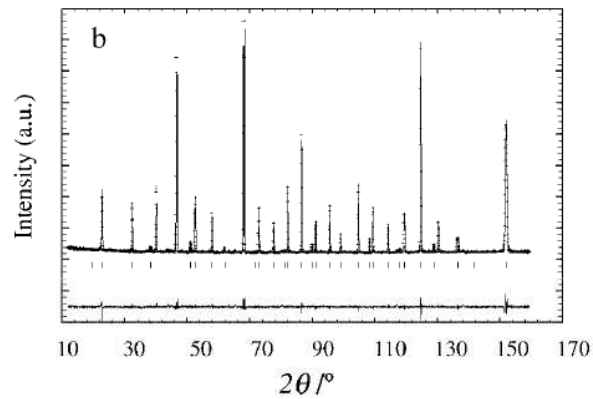


Figure 2. Observed (crosses), calculated (full line) and difference (bottom) high resolution NPD Rietveld profiles for A_2NiMoO_6 collected at 295 K with $\lambda = 1.594 \text{ \AA}$ for (a) A = Sr, (b) A = Ba

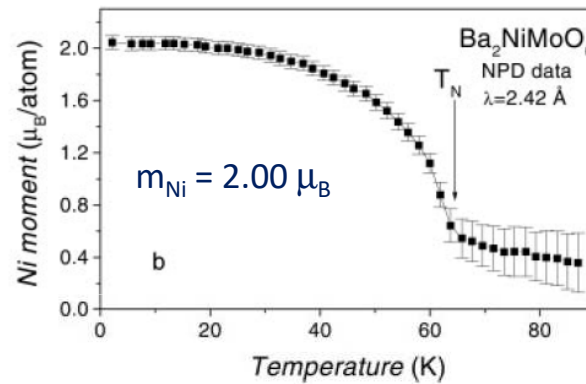


Figure 5. Thermal variation of the ordered magnetic moments for Ni in the antiferromagnetic structure of A_2NiMoO_6 : (a) A = Sr (b) A = Ba

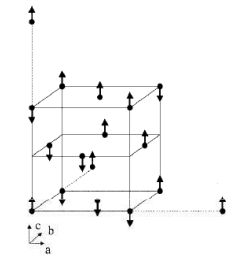
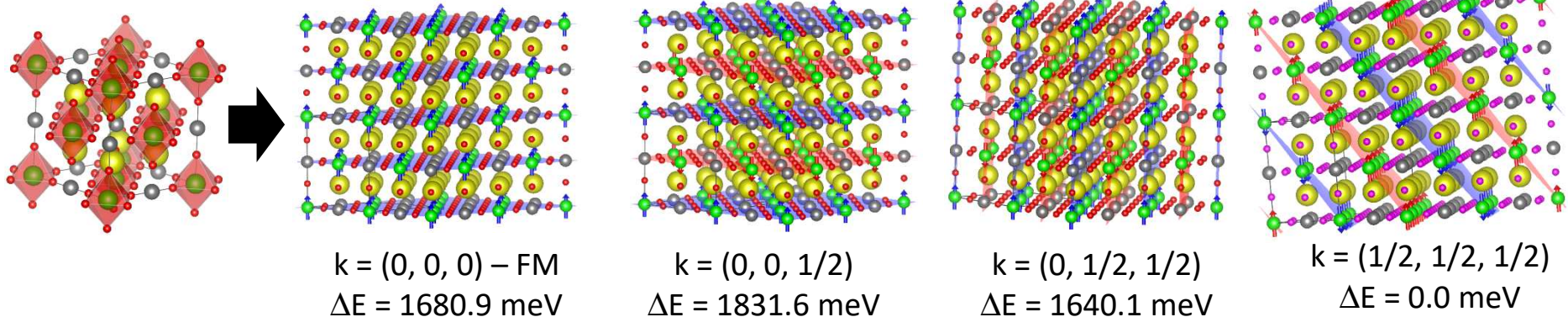


Figure 6. A sketch of the magnetic structures for: (a) Sr_2NiMoO_6 , with $k = (1/2 \ 0 \ 1/2)$; the magnetic unit cell consists of four crystallographic cells, and (b) Ba_2NiMoO_6 , with $k = (1/2 \ 1/2 \ 1/2)$; for the sake of clarity, the figure shows the chemical cell ($a \approx 8 \text{ \AA}$) and part of three adjacent cells

DFT



Inhibition of cyclin-dependent kinase CDK1 by oxindolimine ligands and corresponding copper and zinc complexes

Rodrigo Bernardi Miguel¹ · Philippe Alexandre Divina Petersen² ·

Fernando A. González Zubizarreta³ · Carlos Columbus Olivares³ ·

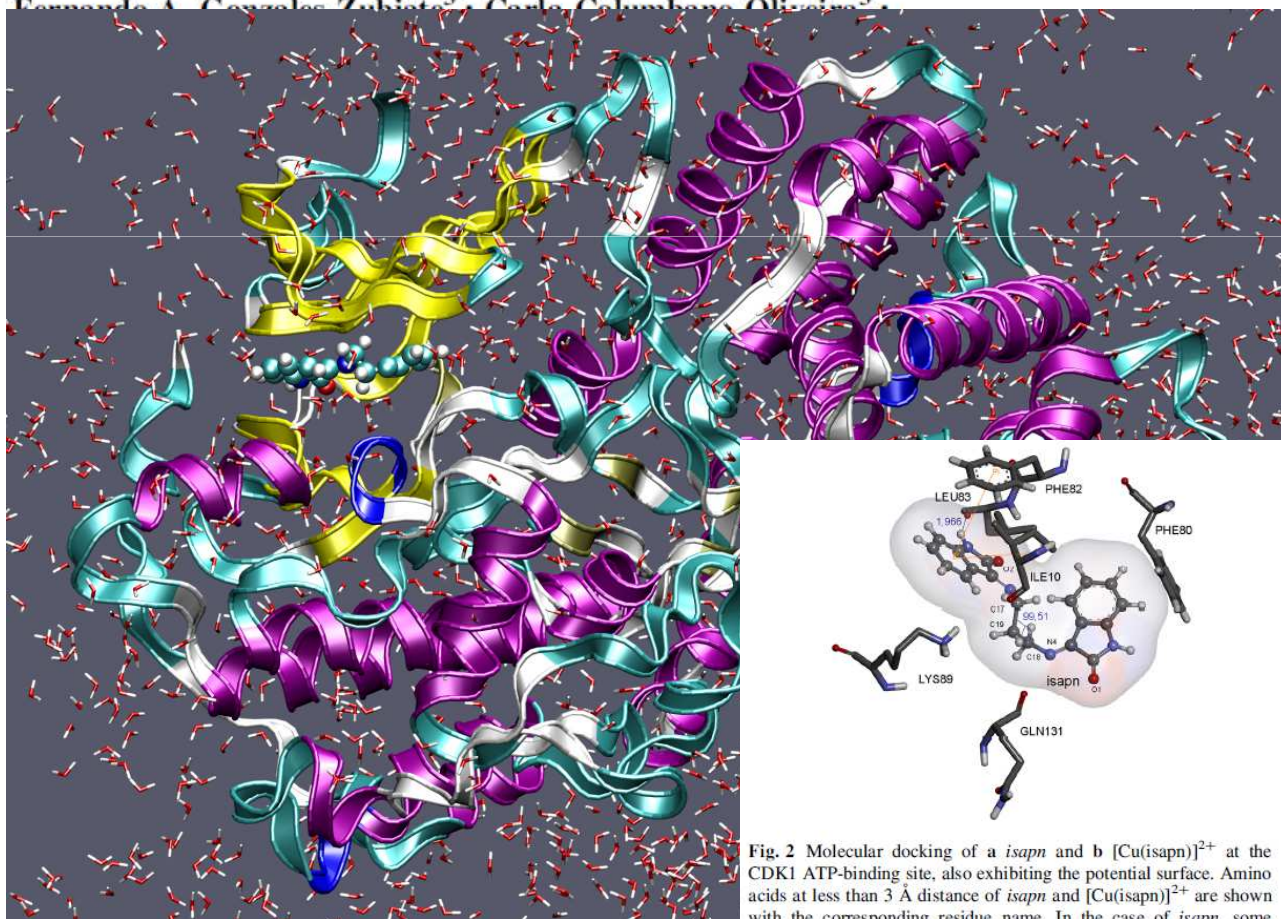
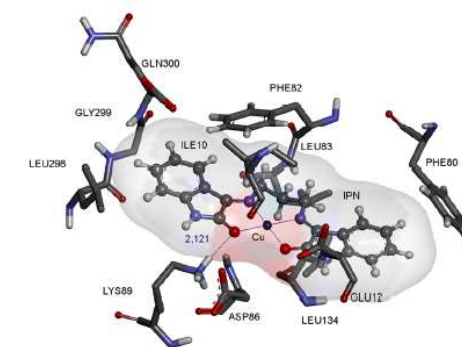


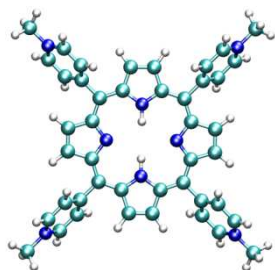
Fig. 2 Molecular docking of a *isapn* and b $[\text{Cu}(\text{isapn})]^{2+}$ at the CDK1 ATP-binding site, also exhibiting the potential surface. Amino acids at less than 3 Å distance of *isapn* and $[\text{Cu}(\text{isapn})]^{2+}$ are shown with the corresponding residue name. In the case of *isapn*, some

Ab-initio Molecular Dynamics (AIMD)

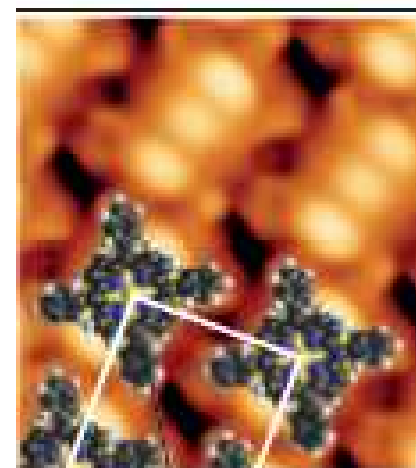
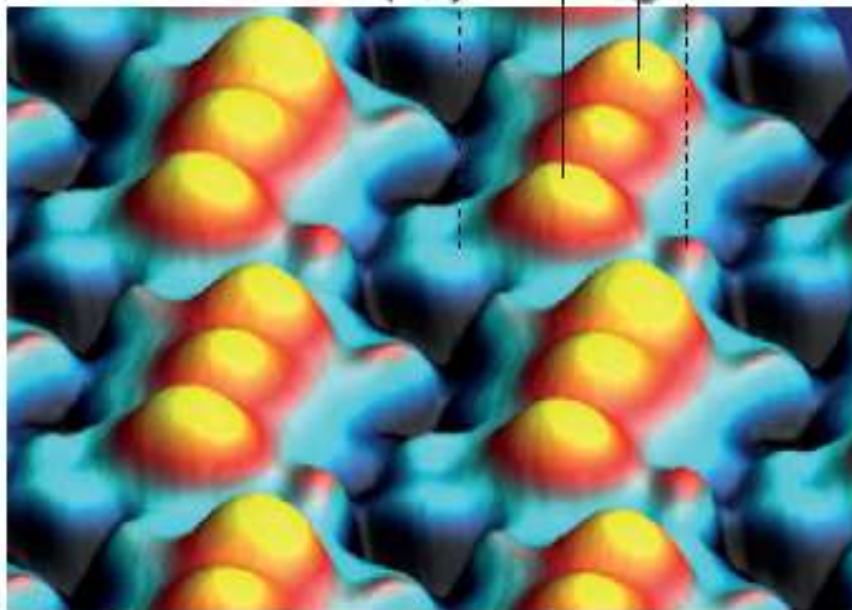
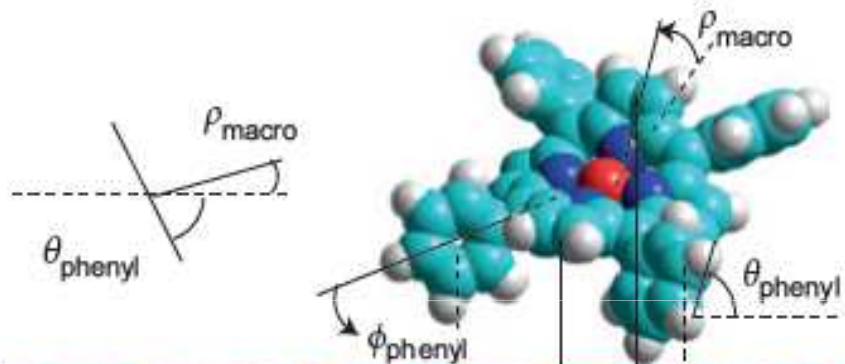


amino acids are omitted for better visualization. *Blue line* the bond distances and torsion angle (dihedral N4–C18–C19–C17). *Yellow lines* the π -stacking interactions (in the case of *isapn*)

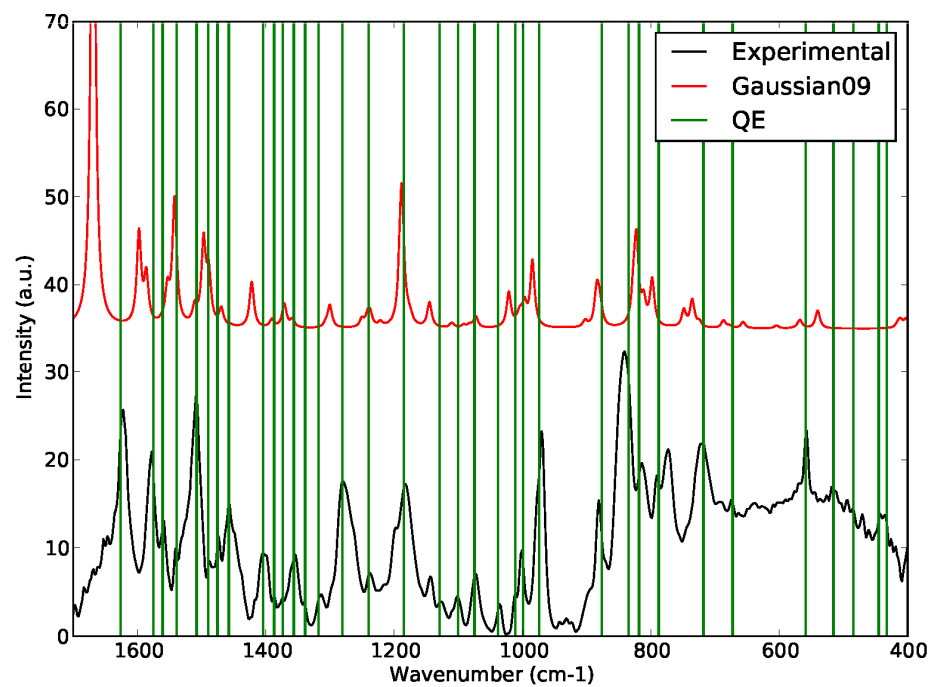
Adsorción de la Porfena TPP sobre superficies metálicas.



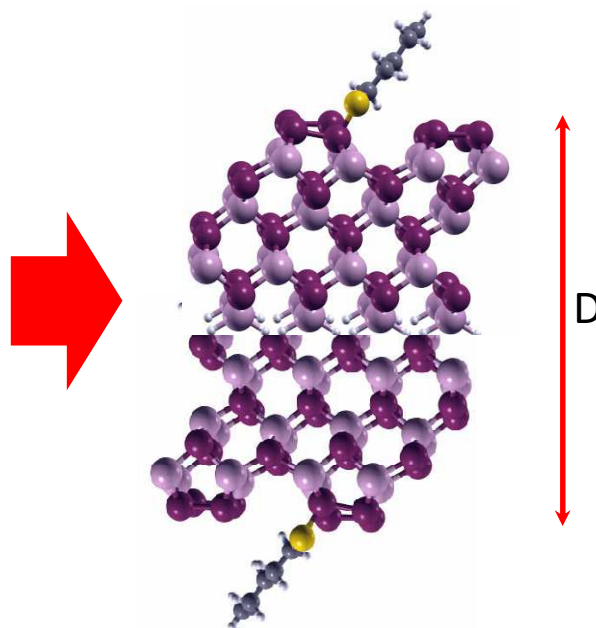
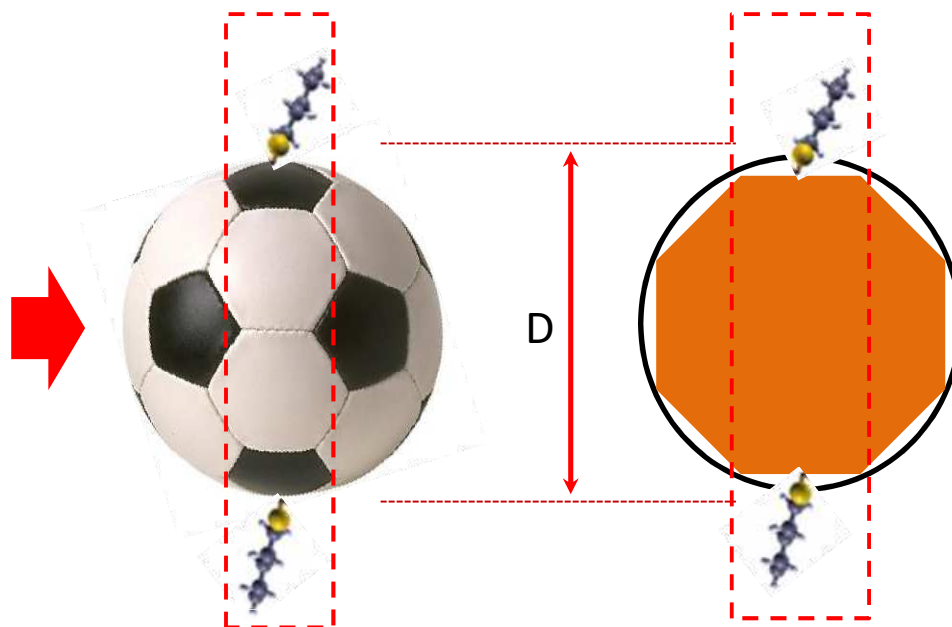
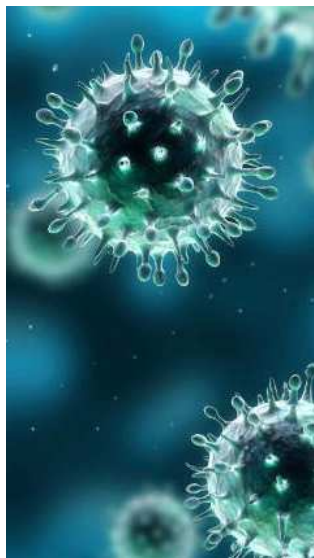
TPP = tetraphenylporphyrin



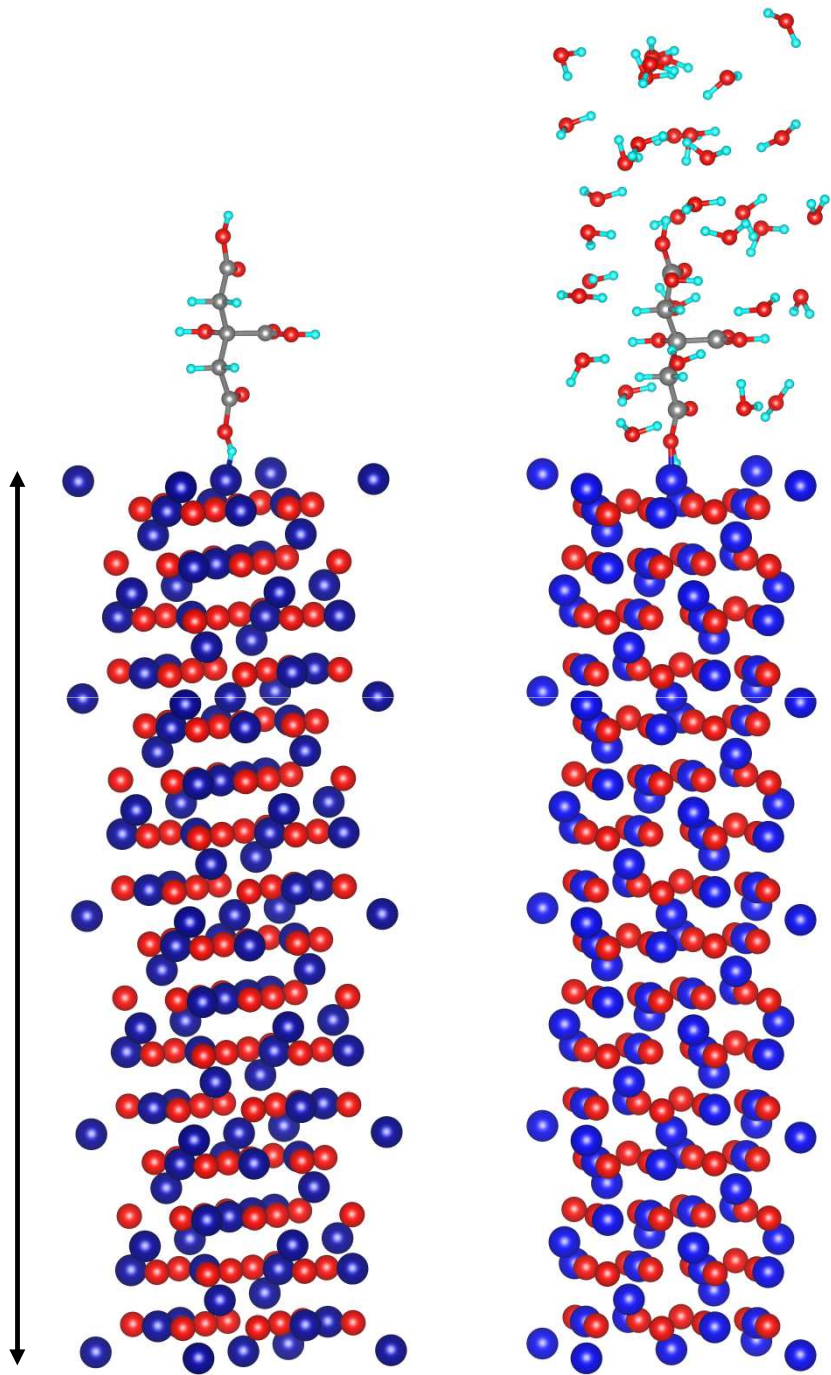
Co-TPP



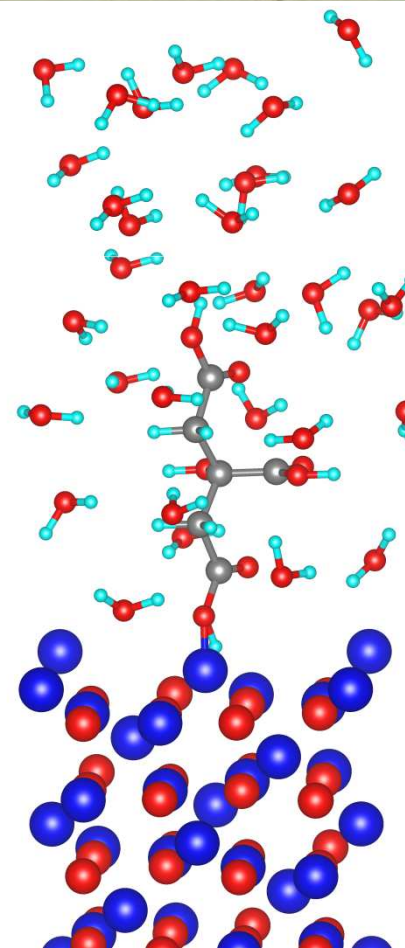
Se puede estudiar nanopartículas?



$\approx 33\text{\AA}$



NP-Fe₃O₄ (magnetita) + C₆H₈O₇



Herramientas necesarias o «Laboratorio»

- Bibliografía.
- Computadoras para hacer los cálculos.
- Internet (buena banda ancha).



Nanomol-N HPC-cluster
Universidad de São Paulo - Brasil



Grendel HPC-cluster
Aarhus University - Denmark



Bluegene -Q Supercomputer
Rice University - USA

Gracias...!!

Acrónimos y siglas

- XANES : X-ray Absorption Near Edge Structure.
- EXAFS : Extended X-ray Absorption Fine Structure.
- VSM : Vibrating Sample Magnetometer.
- SQUID : Superconducting Quantum Interface Devices.
- PAC : Perturbed Angular Correlation Spectroscopy.
- NMR : Nuclear Magnetic Resonance.
- NQR : Nuclear Quadrupole Resonance.
- EPR : Electron Paramagnetic Resonance.
- TPD : Temperature Programmed Desorption.