

## Grupo de Investigación: Química Teórica y Computacional

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Departamento Química Física y Analítica



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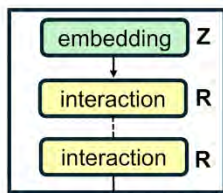
Investigadores en Formación:

Miguel Gallegos González

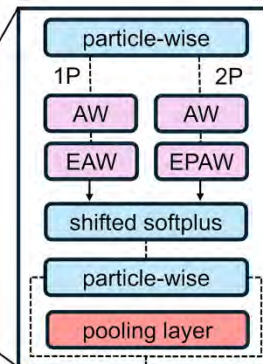
Daniel Barrena Espes

Diogo Jose Lopes Enriques

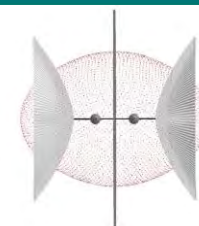
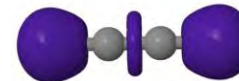
QTCOVI en



SchNet4AIM



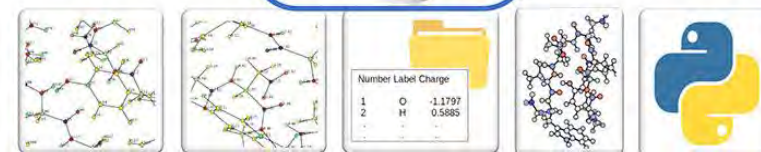
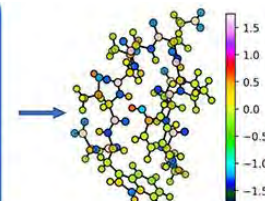
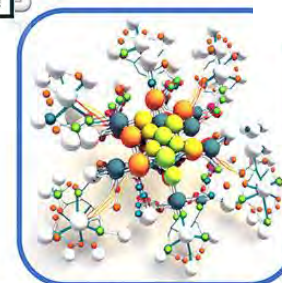
ELF



- ✓ Model creation
- ✓ ML Prediction
- ✓ Equilibration
- ✓ Visualization

- Easy-to-use.
- Flexible architecture.
- Python based.
- Custom models.

NNAIMGUI



Redes neuronales y descriptores

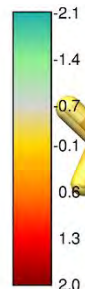
*Desarrollo y validación de metodologías químico-computacionales y de software avanzado para su aplicación.*

Interacting Quantum Atoms

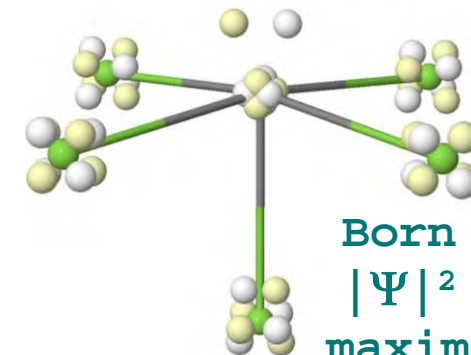
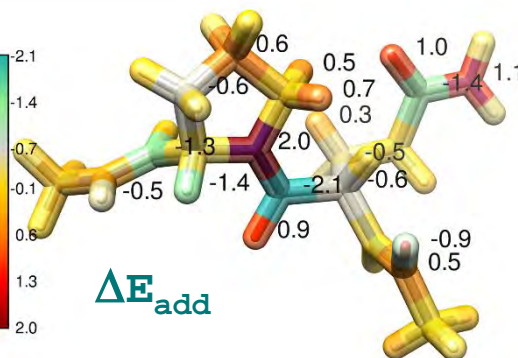
PROMOLDEN

```

# ----- PROMOLDEN -----
# --- MOLECULAR PROPERTIES OF SCALAR DENSITY
# --- Version 1.80
# --- (c) E. Francisco
# --- A. Martín Pendás
# --- J. L. Casals-Sainz
# --- University of Oviedo, Abril, 20
# -----
    
```



$\Delta E_{add}$

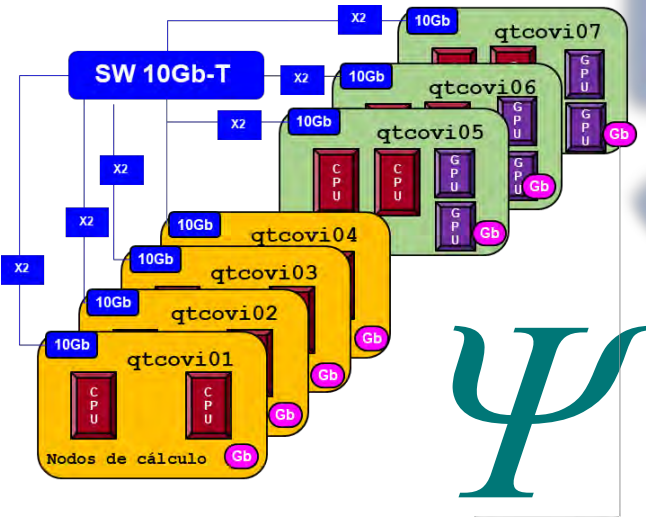


Born  
 $|\Psi|^2$   
maxima

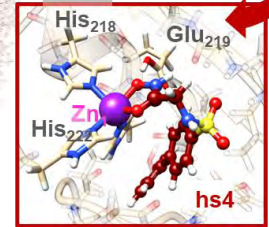
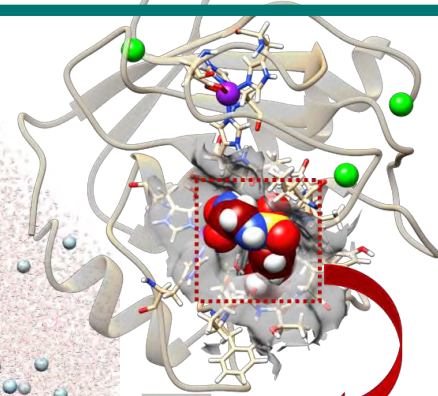
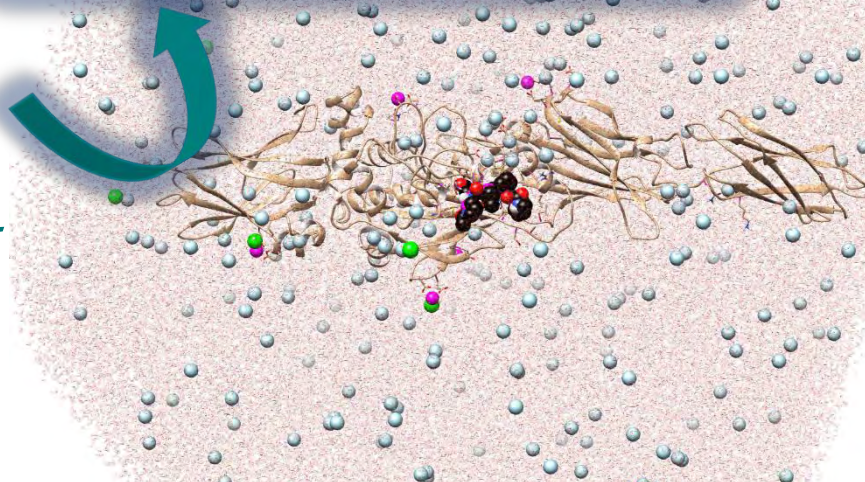
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# ----- PROMOLDEN -----
# --- MOLECULAR PROPERTIES OF SCALAR DENSITY
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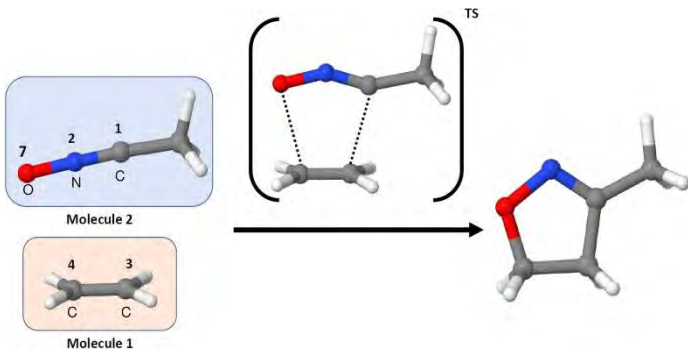
QTCOVI en C3



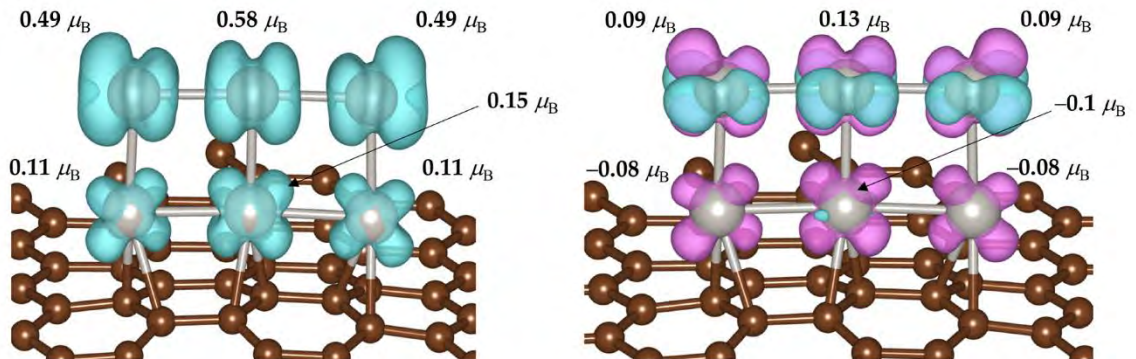
*Simulación molecular de alto nivel de sistemas y procesos moleculares de especial interés.*



Biomoléculas



Reactividad y propiedades químicas

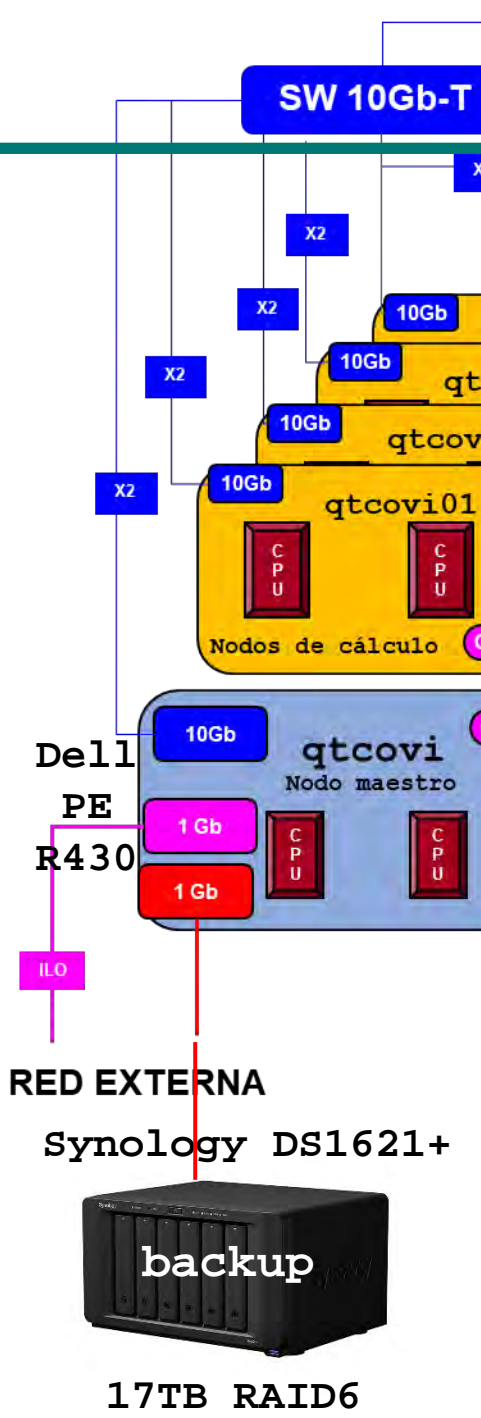


Pt<sub>6</sub>-I  
 $\Delta E = 0.0$  eV  
 $\mu = 1.9 \mu_B$

Semiconductores y catalizadores

Pt<sub>6</sub>-I'  
 $\Delta E = 0.09$  eV  
 $\mu = 0.0 \mu_B$

**HARDWARE**



Servidor	CORES	RAM	HD1	HD2	GPU
Lenovo SR630	64	512GB	484GB SSD	3.5 TB SSD	0
Supermicro 6029U-TRT	96	385GB	431 GB SSD	3.8TB NVMe	0
Supermicro 6019U-TNRT	96	385GB	196GB NVMe	3.8TB NVMe	0
Supermicro 1029GQ-TNRT	96	385GB	196GB NVMe	3.8TB NVMe	2 RTX5000
Supermicro 1029GQ-TNRT	96	385GB	196GB NVMe	3.8TB NVMe	2 RTX5000
Supermicro 1029GP-TR	96	385GB	984GB NVMe	3.8TB NVMe	2 A100

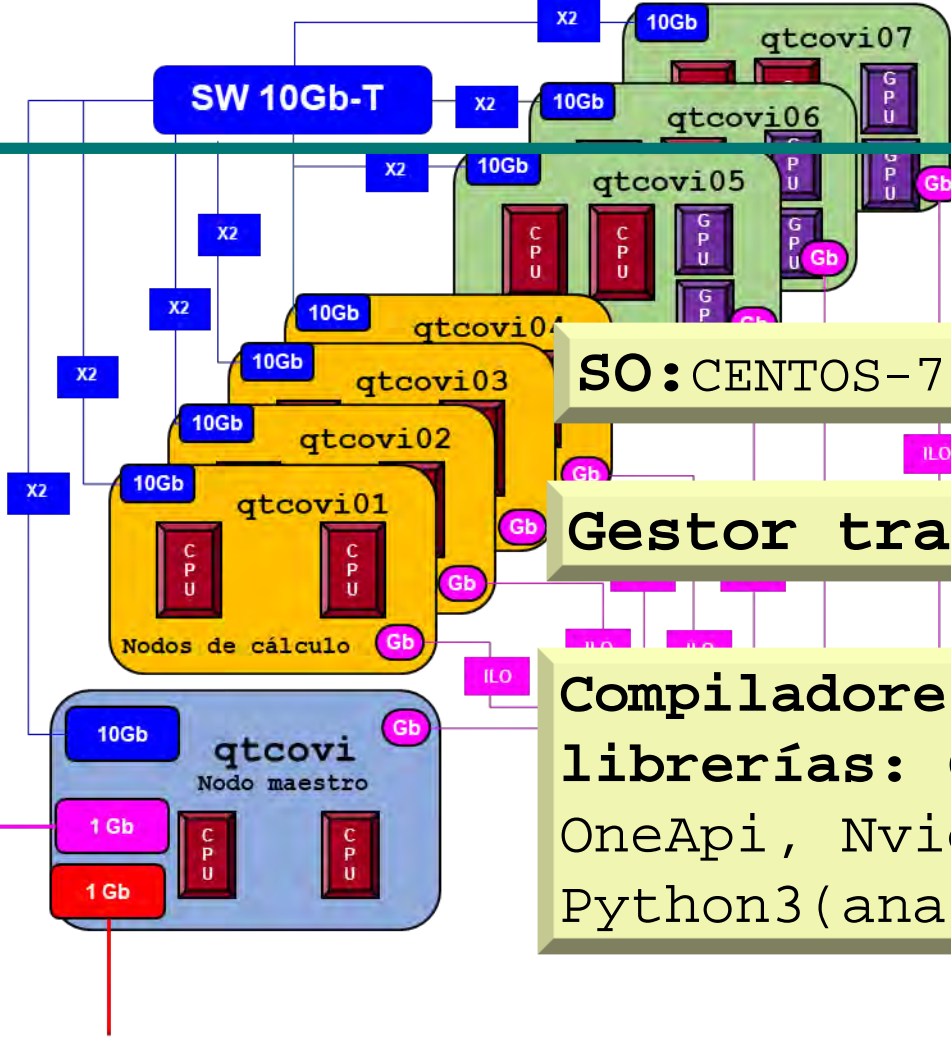
## SOFTWARE

**SO:** CENTOS-7 → Update AlmaLinux 8

**Gestor trabajos:** torque 6.1.2

**Compiladores, intérpretes, librerías:** GNU 8.3, Intel OneApi, Nvidia HPC\_SDK, Python3(anaconda), etc.

**Toolbox:** aimall, pyscf, psi4, chimera, dftd3, multiwfn, vmd, **amber23**, gamess, namd, **orca**, xtb, quick, denmat, **gaussian16**, jmol, molden, **promolden**, **vasp**, etc.



RED EXTERNA

