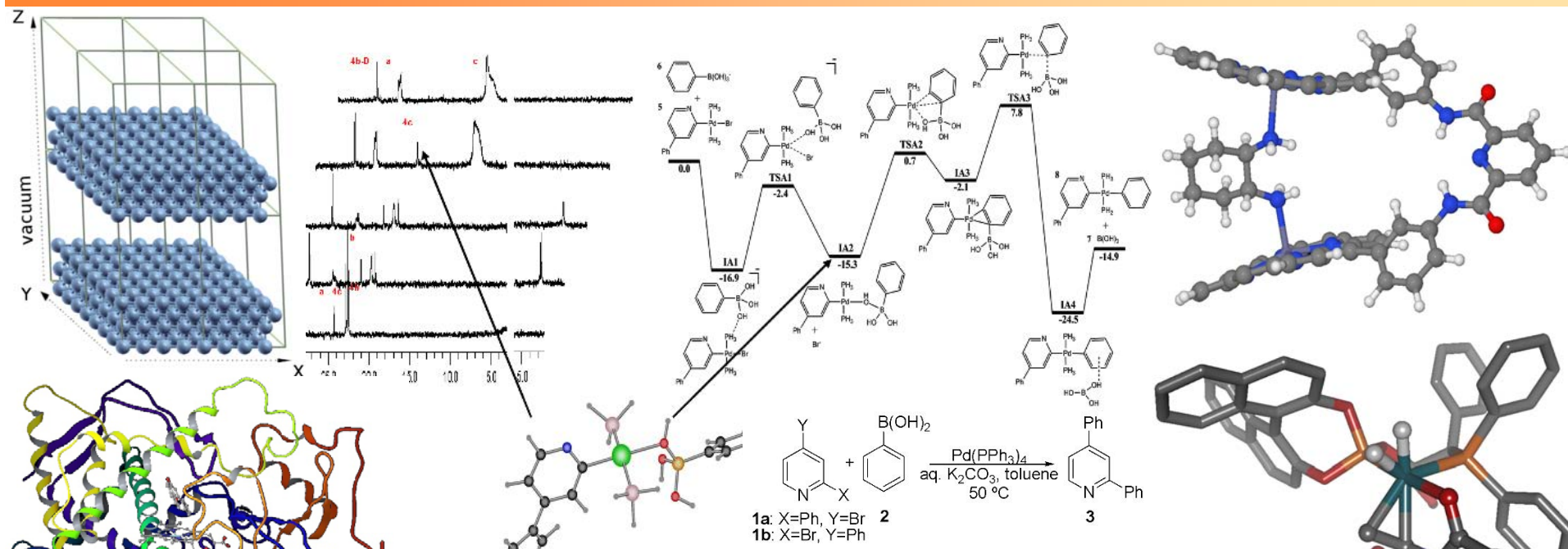
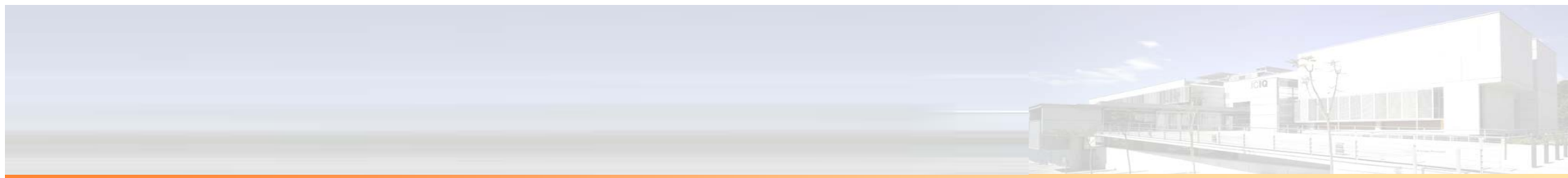
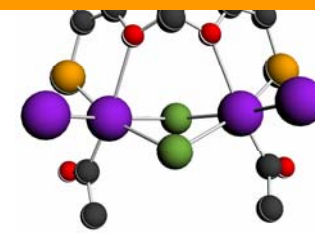
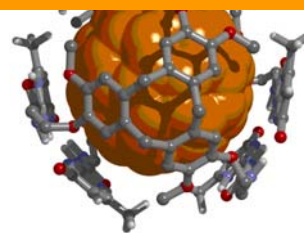
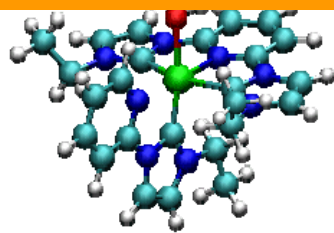
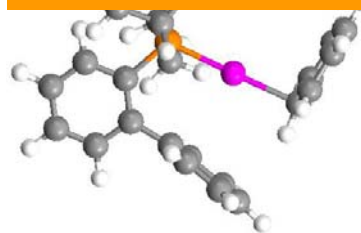
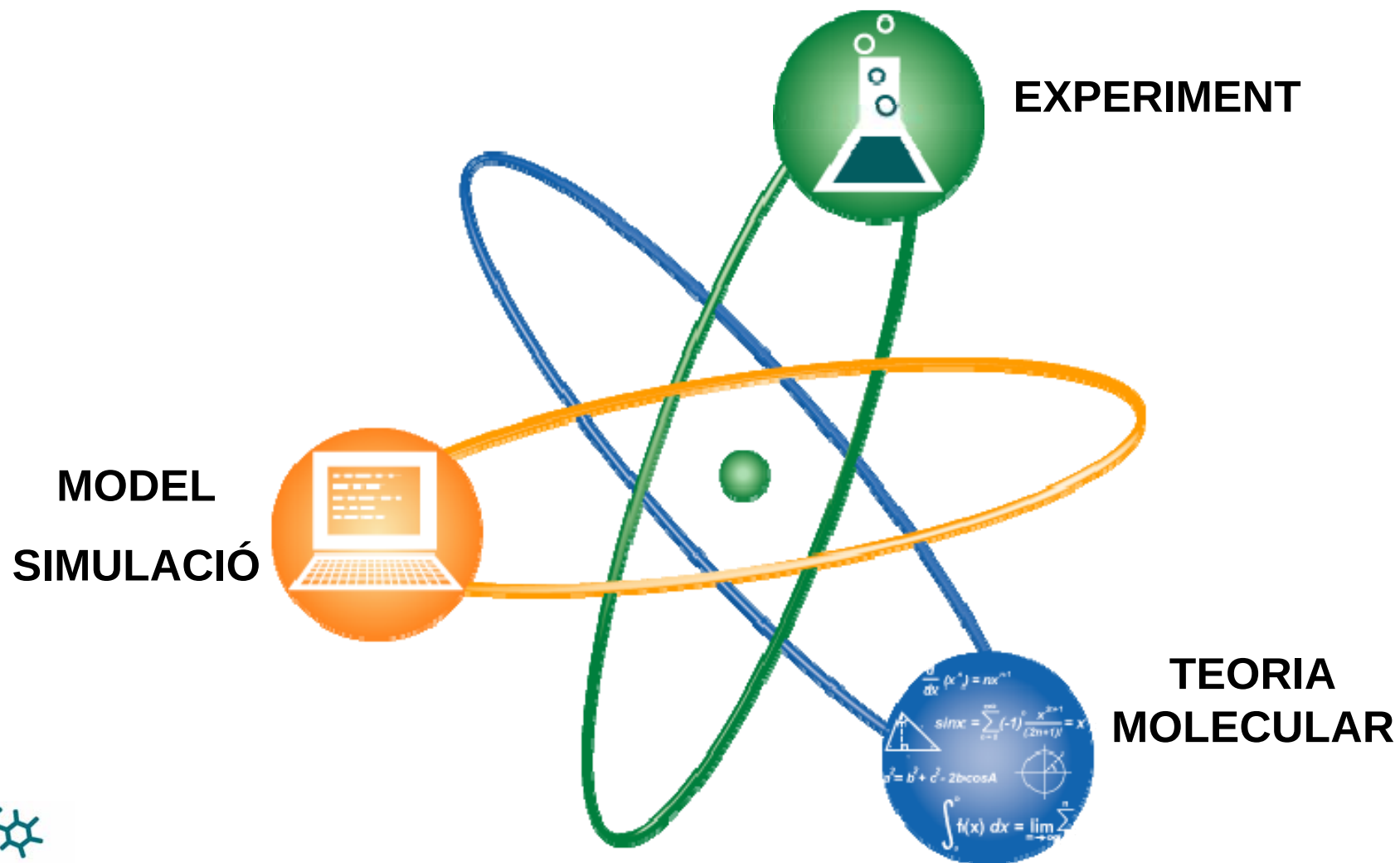
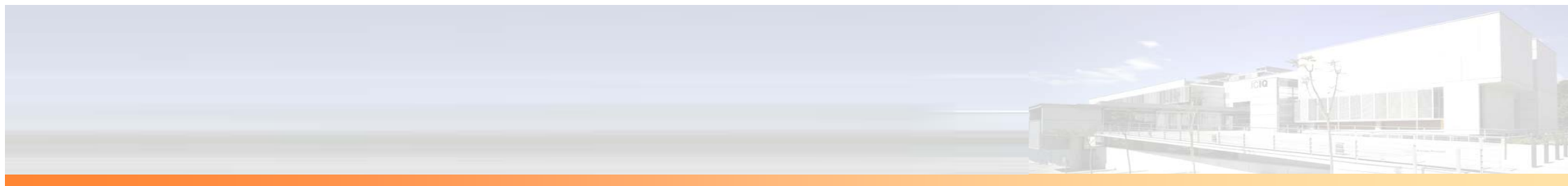




Laboratori de Química Computacional





Avantatges de la simulació

- **Validació de la teoria i del model**
- **Cost** reduït comparat amb la realització d'experiments
- **Seguretat**: ni toxines, ni residus, ni materials inestables,...
- **Precisió** és usualment alta
- **Comprensió de la realitat**
- **Disseny de nous materials**

Supercomputadors

ICIQ

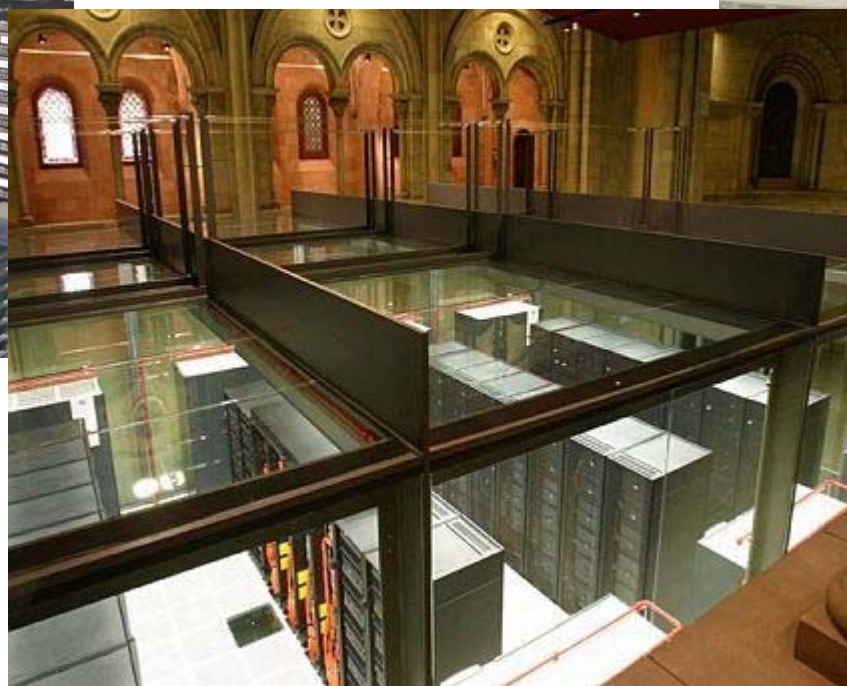


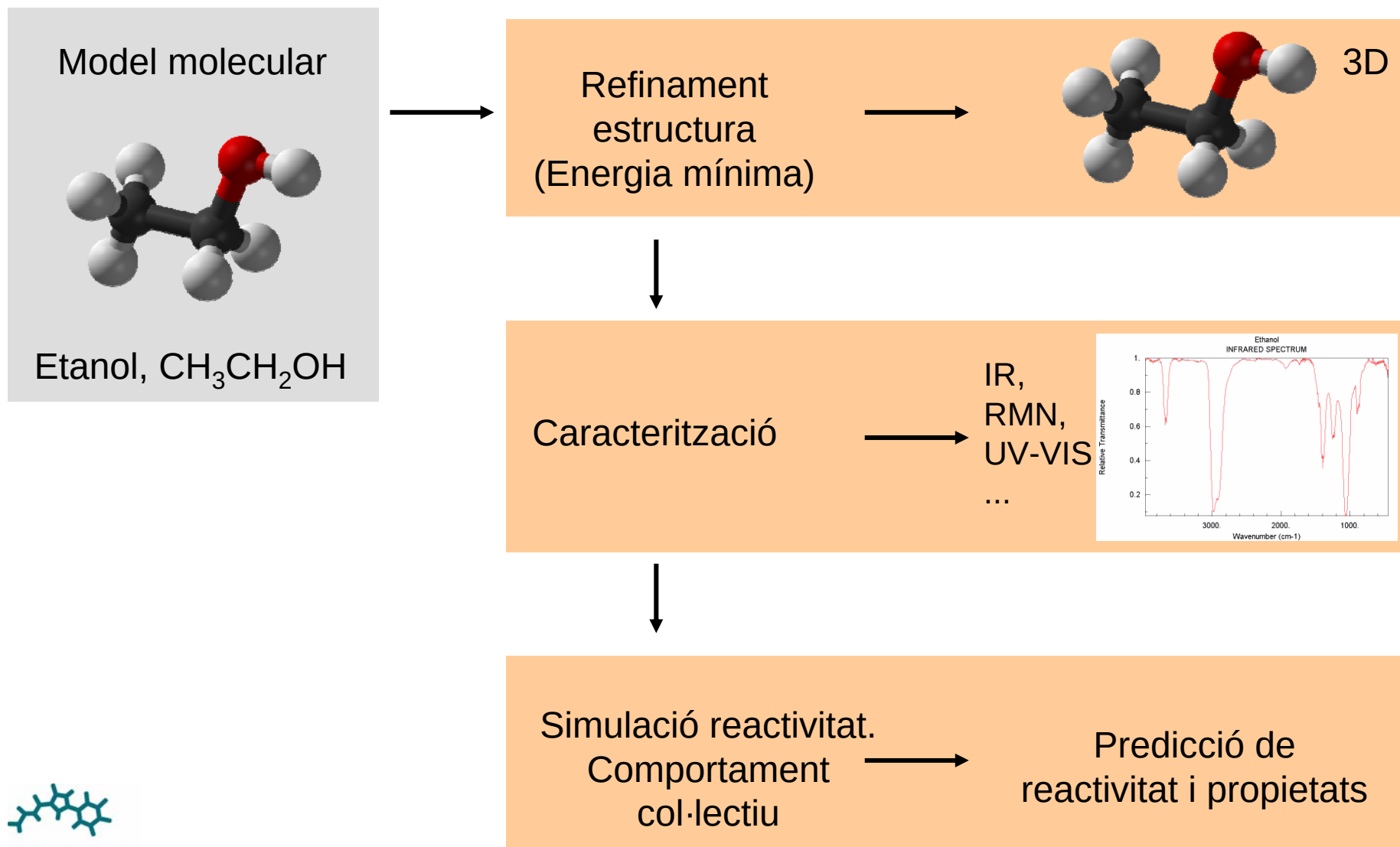
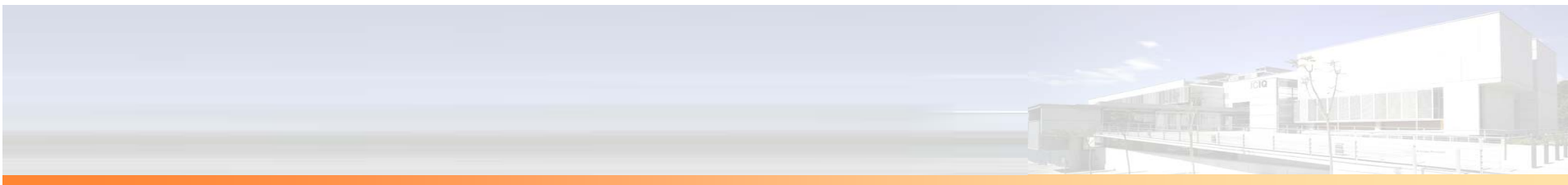
CESCA

(Centre de Supercomputació de Catalunya)

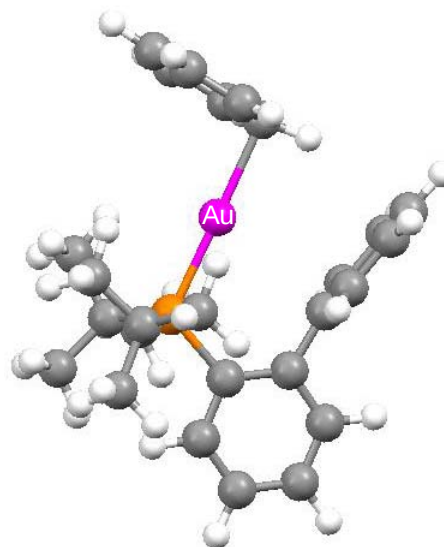
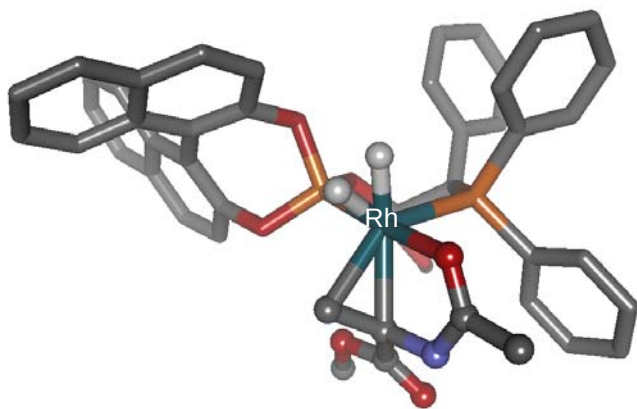
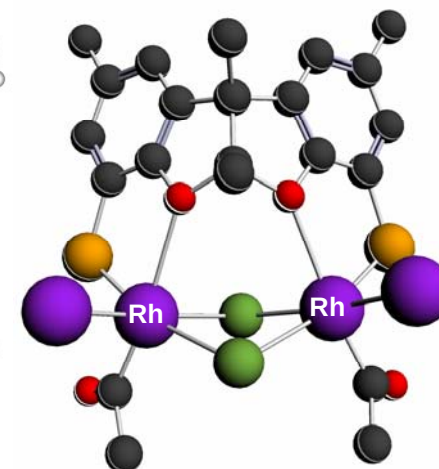
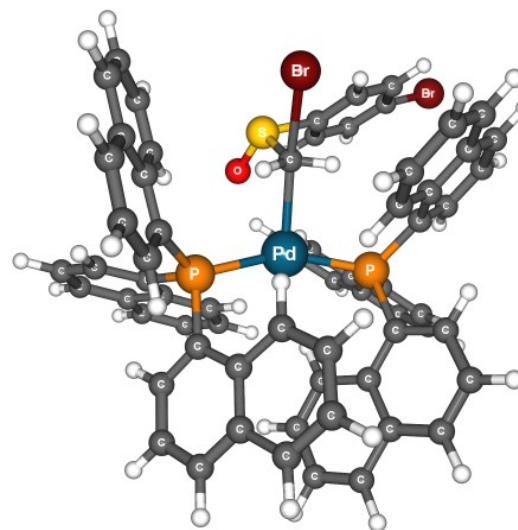
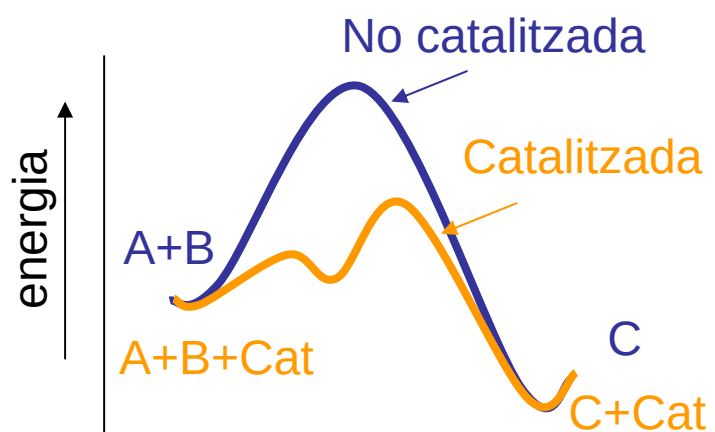


Marenostrum
(Barcelona
Supercomputing Center)

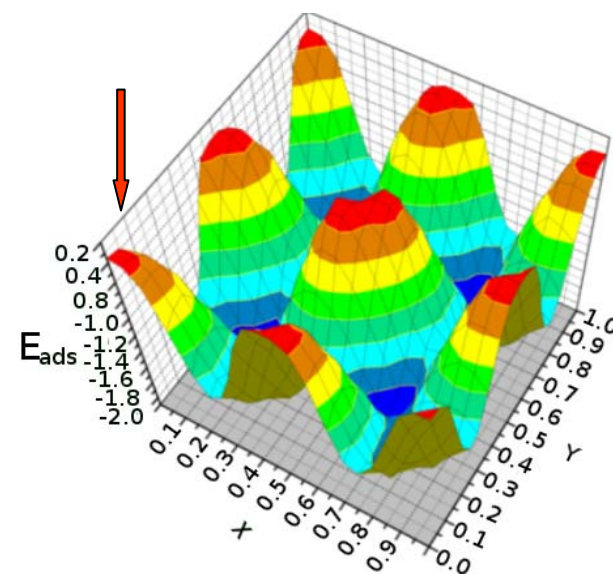
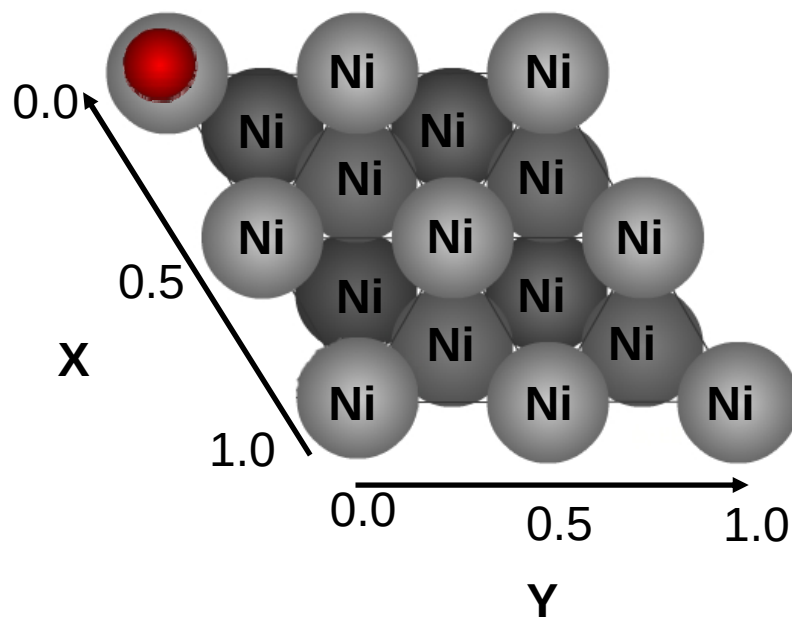




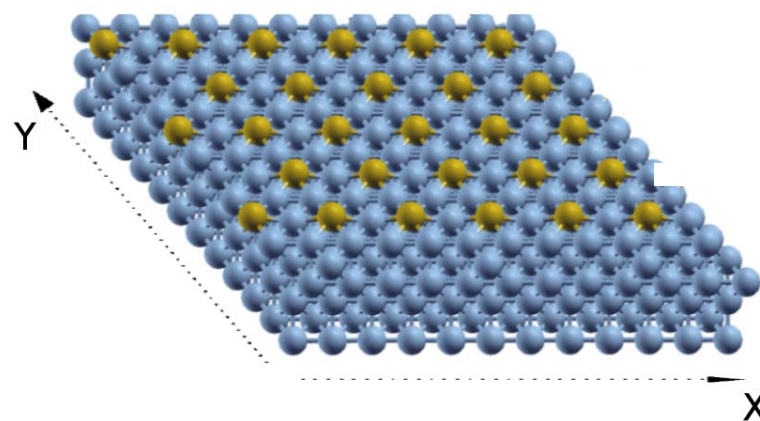
Què fem?



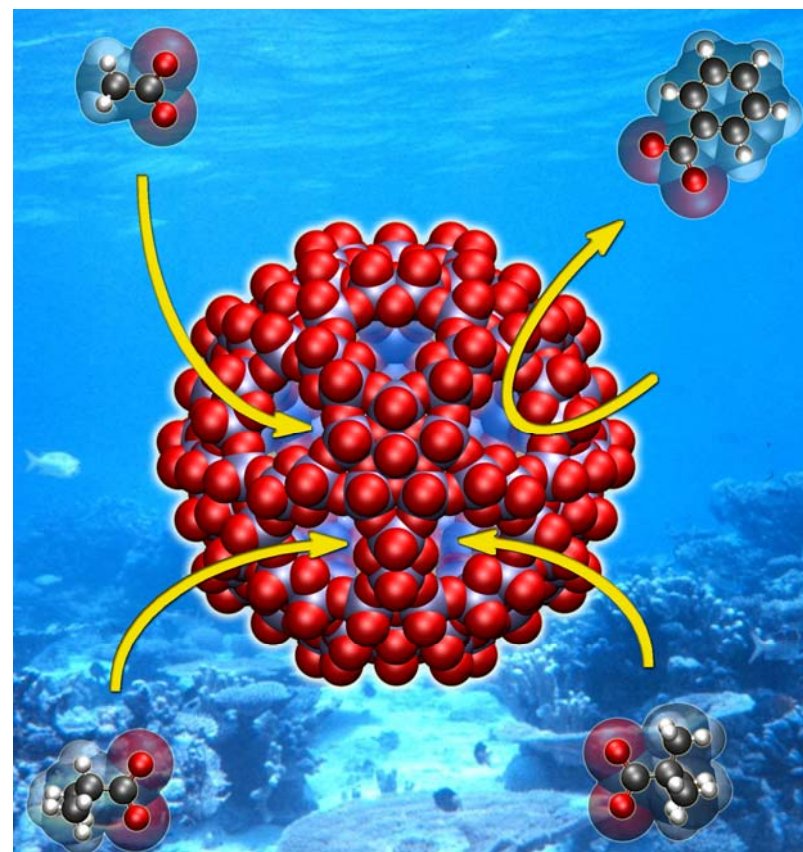
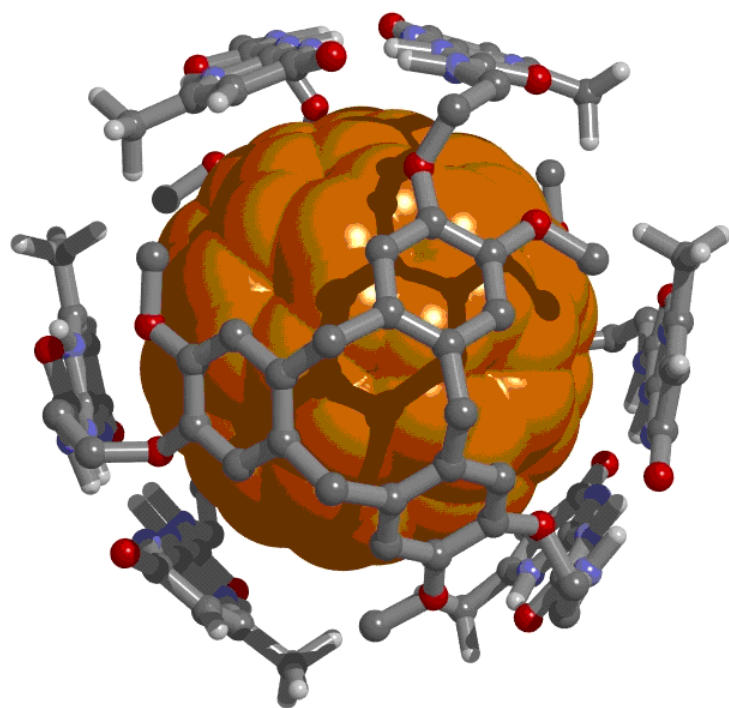
Què fem?



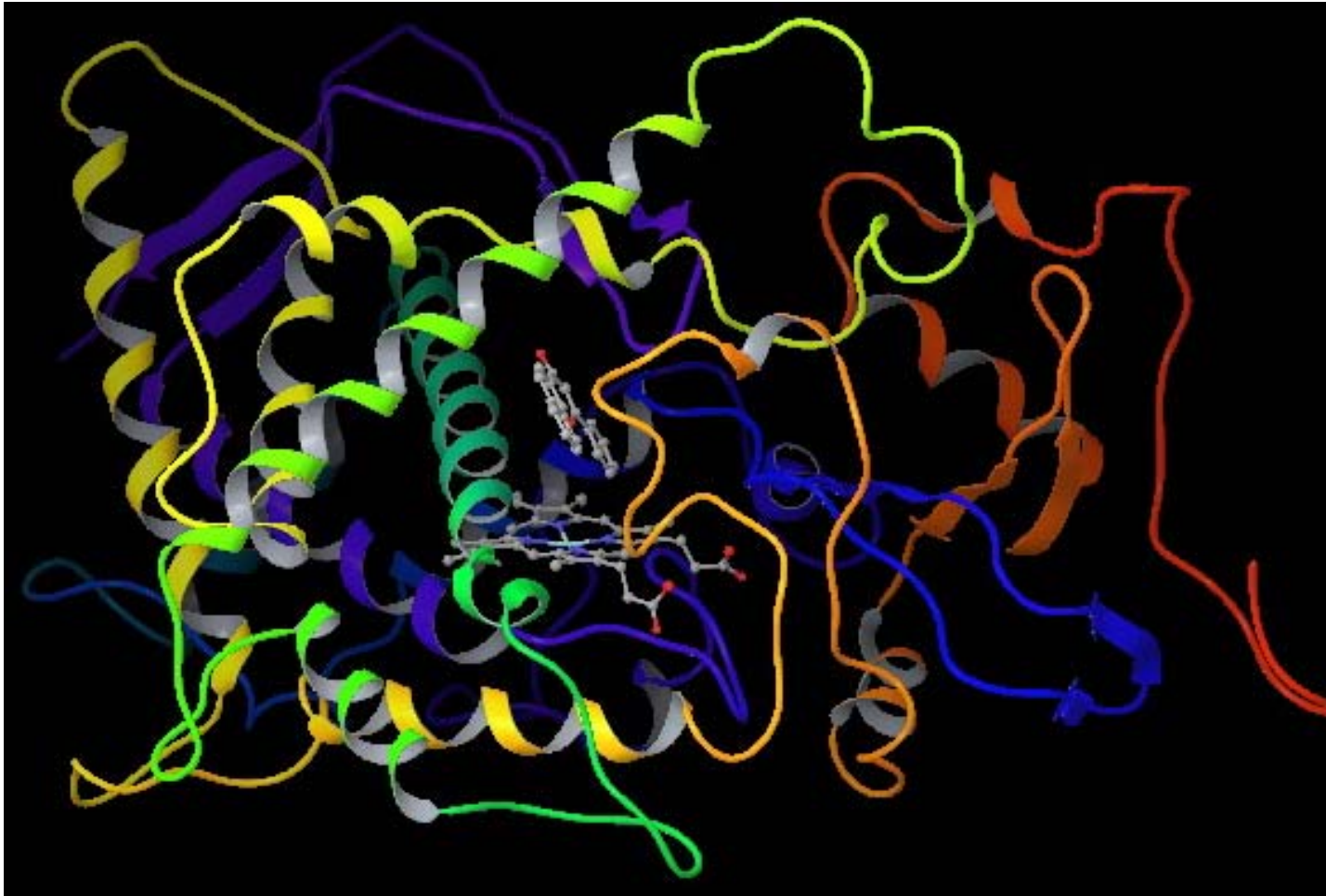
Aliatge AuNi_3

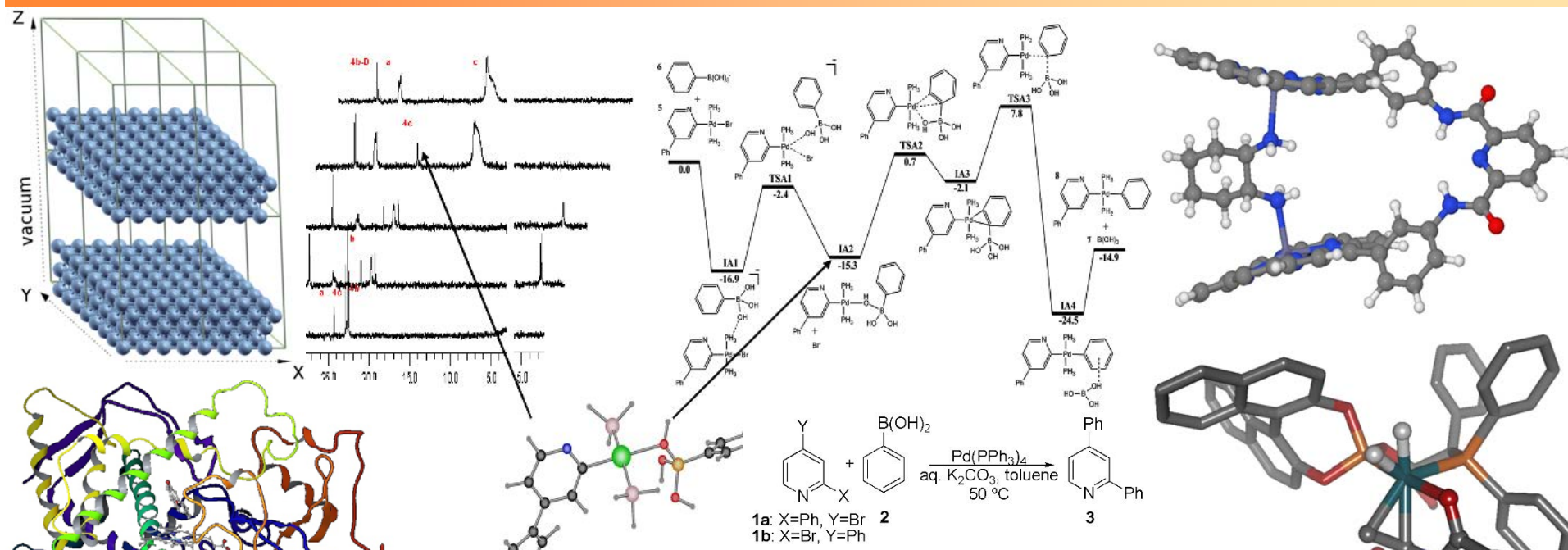
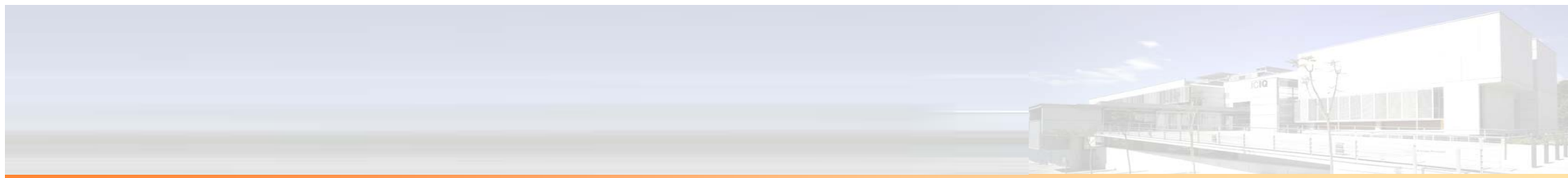


Què fem?



Què fem?





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