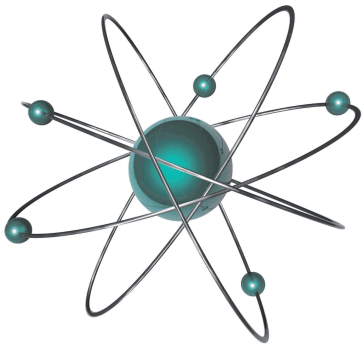
Reference Network on
Theoretical and Computational Chemistry



Prediction of polymorphs in crystalline systems with technological potential

The identification and characterization of all the possible crystalline polymorphs is of great interest in fields such as the development of new drugs. Theoretical prediction of polymorphs is an extremely valuable complementary tool since it allows synthesis experiments to be undertaken that are targeted specifically at obtaining genuine new polymorphs, whose structure has previously been discovered in virtual simulations.

Who is it aimed at?

- Companies in the pharmaceutical sector
- Companies in the chemical industry
- Research groups

What is it for?

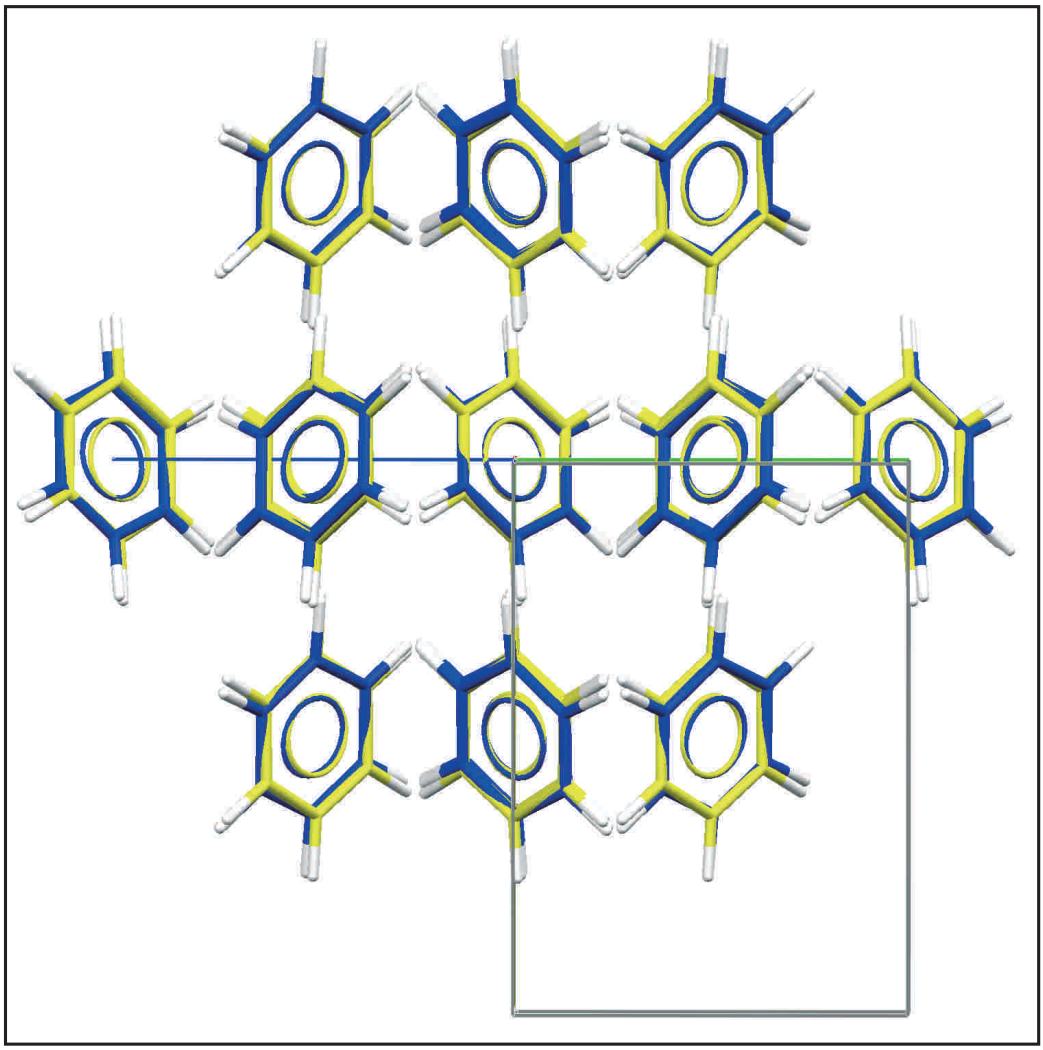
- The prediction of crystalline structures is a very powerful tool for **gaining an understanding and predicting the pharmacological, optical or magnetic properties of molecular crystals.**

- Each **crystalline polymorph can be individually patented**, therefore the prediction of new polymorphs, and their later synthesis, potentially generates **new patentable materials** from compounds that are already patented and being commercialized, or can be the first step in a process of registering the first patent of the compound.

Description of the technology

• The code developed for the prediction and optimization of crystals, PixCryPar, is an MPI-paralellized version that allows **crystalline structures to be predicted** in the most likely spatial groups, at a very reasonable computational cost.

• In order to satisfactorily make a prediction, the interactions within the crystal are described in precise detail; that is, the intermolecular interactions. In PixCryPar these interactions are described by potentials of new generation, known as pixel-potentials, which are based on concentrating the previously calculated molecular electron density ab inicio into a given volume or pixel, and calculating the intermolecular energy as the sum of the interactions between pixels. This allows a very precise description of the intermolecular energy for any molecular crystal or co-crystal.



Comparison of the experimental structure and the calculated structure for one of the polymorphs of the benzene crystal.

For further information: **(+34) 93 402 02 41**
xrqtc@fbg.ub.es **www.xrqtc.com**

Generalitat de Catalunya
Departament d'Innovació, Universitats i Empresa
Comissionat per a Universitats i Recerca

Fundació Bosch i Gimpera
Universitat de Barcelona