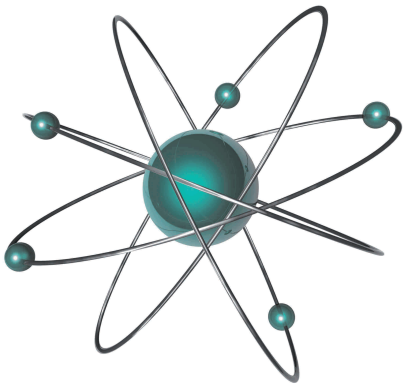
Reference Network on
Theoretical and Computational Chemistry



DESIGN AND OPTIMIZATION OF CATALYSERS FOR enantioselective processes via quantum-mechanical calculations

Who is it aimed at?

- The pharmaceutical industry
- The fine chemistry sector

What is it for?

- Computational chemistry can at present predict with reasonable precision the **enantiomeric excess of homogenous catalytic processes.**

- The **effect of a modification to the catalyser** on selectivity can be predicted a priori without the need to synthesize the modified compound in the laboratory.

- This method can be used to **design more efficient catalysers or catalysers that can treat particularly tricky substrates.**

Description of the technology

- **It is compatible with a great variety of methods** for producing thin films (evaporation techniques as well as drop-casting or spin-coating processes) and Langmuir-Blodgett films.

- They can be absorbed into a nanocrystalline semiconductor or anchored in polymeric substrates without aggregation.

- **No parameterization is required**: no empirical or semi-empirical data are necessary.

- **It avoids the alignment stage** that is necessary in many CoMFA approximations, and which require knowledge of the interactions between the catalyser and the substrate, and can be problematic with structures that are highly flexible.

- **It successfully predicts R- and S-configurations.**

- **It successfully predicts enantiomeric excesses.**

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