

Post doc position on nucleation resulting in symmetry breaking (12 months)

Enantiomer separation is very important for the pharmaceutical industry, because active pharmaceutical ingredients are often chiral and mostly only one of the enantiomers exhibits the required pharmaceutical activity. Therefore, to increase drug efficacy and to comply with the requirements of the regulatory authorities, enantiomers need to be separated.

The SMS laboratory is specialised in the development of separation methods of chiral compounds **by crystallisation**.

Crystallisation methods are often sought after by companies (because the process is easily scaled up to industrial quantities with a high degree of purity for crystalline compounds); however, their principal difficulty is finding the specific crystallisation conditions to obtain enantiopure crystals. It is difficult to obtain these parameters, because crystallisation of new compounds is quasi impossible to foresee in spite of existing theoretical models and computer simulations. In particular nucleation, the first step in crystallisation, is not well understood and is not controlled within crystallisation processes and should be studied in more detail.

The scientific objective of this research project is therefore **to study the mechanisms of nucleation in particular of chiral molecules or of compounds that present a supramolecular chirality to improve our understanding (and ideally to predict) the identity of the phase obtained after crystallisation.**

After Viedma had demonstrated that it was possible to obtain symmetry breaking in a solution by an attrition mechanism, our group has published about an improved method that uses temperature cycles to induce the deracemization. Subsequently, we have actively contributed to the knowledge and the development of the symmetry breaking method.

The post-doctoral researcher will work with well-characterized molecular models from our laboratory with the objective to control the appearance of conglomerates. In addition, the researcher will establish the conditions under which symmetry breaking will occur to obtain a 100% yield. At present, several molecules are in the process of being synthesized in the laboratory with the aim to be used for symmetry breaking studies. For each system, we will precisely determine the conditions of conglomerate formation. Racemic mixtures will be studied by vibrational circular dichroism (VCD) to observe the start of nucleation and to better understand the crystallization conditions of enantiopure crystals. The effect of polarized light on the enantiomer that crystallises will be studied too.

The candidate for the post-doc position must have a PhD in chemistry, physical chemistry, or physics with a specialization in physical chemistry, analytical chemistry or solid-state analysis. Having experience with calorimetric measurements, X-ray diffraction or surface analysis is a plus. Knowledge of crystal growth, nucleation, and phase diagrams will be appreciated.

Period: 12 months

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