

Exploring Structures and Structural Phenomena: The Derived Crystal Packing Model

Claire Gervais^a, Morgan Pauchet^b, Gérard Coquerel^b, ^a *Department of Chemistry and Biochemistry, University of Bern, Switzerland.* ^b *UC²M², University of Rouen, France.* E-mail: claire_gervais@hotmail.com

Improvements in the prediction and the design of molecular crystals have been dramatically enhanced the last decades. However, several problems during crystallization such as polymorphism or two-dimensional defects can lead to difficulties in interpreting the success of a theoretical study.

In this context, we developed the Derived Crystal Packing (DCP) model [1]. This two-step procedure allows to generate crystal structures (daughter phases) starting from periodic fragments retrieved from a known mother phase. The study of many examples has shown that concomitant polymorphism, twinning and epitaxies can be a direct consequence of the structural and energetical similarities between the mother and the daughter phases.

These issues will be illustrated by the case of (\pm) Modafinil, a pharmaceutical compound known to crystallize in several polymorphic forms and solvates [2].

[1] Gervais C., Coquerel G., *Acta Cryst. B*, 2002, **58**, 662. [2] Pauchet M., Gervais C., Courvoisier L., Coquerel G., *Cryst. Growth. Des.*, 2004, **4**, 1143-1151.

Keywords: crystal structure prediction, twinning, polymorphism