

W0045

Designing Molecular Interfaces. Colin C. Seaton, N. Blagden, Drug Delivery, School of Pharmacy, Univ. of Bradford, Bradford, UK, c.seaton@brad.ac.uk

A key aim of crystal engineering is the design and synthesis of new materials with defined functionality through the control of intermolecular interactions. The formation of hybrid materials, created from two separate crystalline components bound through some epitaxial interface, are of interest since the properties can be controlled through selection of components. Design of these systems requires an understanding of the bonding relationships between the layers. Traditionally, this is achieved by a geometric analysis of the components, however this does not consider the role of supramolecular synthons at the interface. To achieve a full understanding a molecular modelling approach is required.

Benzoic acid and benzamide were selected as a test system due to similarities between the crystal structures and complementary nature of the hydrogen bond donor and acceptor groups on each molecule. Models were created from the known crystal structures and the differential evolution¹ algorithm was applied to minimise the lattice energy. We will show the initial results of both computational and experimental studies into this system.

K.V. Price (1999) *An introduction to differential evolution* in *New Ideas in Optimisation*, D. Corne, M. Dorigo, F. Glover (Eds), McGraw-Hill, London UK.