Keynote Lecture

KN23

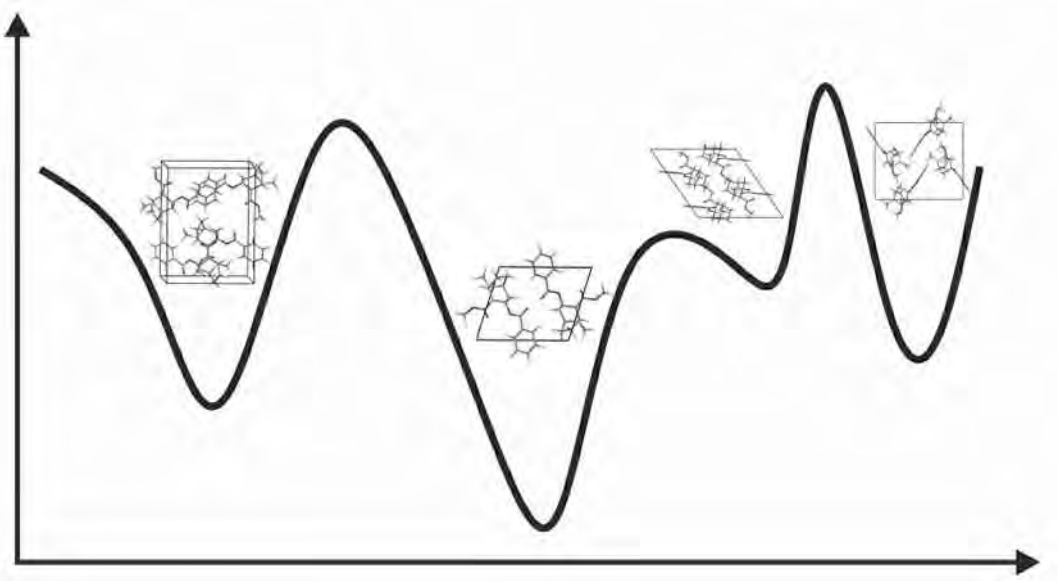
Insight from energy surfaces: structure prediction by lattice energy exploration

G. Day[1]

[1]*University of Southampton, Chemistry, Southampton, United Kingdom*

A long-standing challenge for the application of computational chemistry in the field of crystallography is the prediction of crystal packing, given no more than the chemical bonding of the molecules being crystallised. Recent years have seen significant progress towards reliable crystal structure prediction methods, even for traditionally challenging systems involving flexible molecules and multi-component solids [1]. These methods are based on global searches of the lattice energy surface: a search is performed to locate all possible packing arrangements, and these structures are ranked by their calculated energy [2]. One aim of this lecture is to provide an overview of advances in methods for crystal structure prediction, focussing on molecular organic crystals, and highlighting strategies that are being explored to extend the reach of these methods to more complex systems. A second aim is to discuss the range applications of crystal structure prediction calculations, which have traditionally included solid form screening, particularly of pharmaceutically active molecules, and structure determination. As energy models become more reliable at correctly ranking the stability order of putative structures, and the timescale required for structure searching decreases, crystal structure prediction has the potential for the discovery of novel molecular materials with targeted properties. Prospects for computer-guided discovery of materials will be discussed.

[1] *D. A. Bardwell, C. S. Adjiman, Y. A. Arnautova et al, Acta Crystallographica, 2011, B67, 535-551.,* ***[2]*** *G.M.Day, Crystallography Reviews, 2011, 17, 3-52*



Keywords: crystal structure prediction, crystal engineering, modelling