VisualHabit: Molecular Modelling of Crystals

ADVANCED DIGITAL DESIGN OF PHARMACEUTICAL THERAPEUTICS

J.H.Pickering, I.Rosbottom, R.B.Hammond & K.J.Roberts
Centre for the Digital Design of Drug Products, School of Chemical and Process Engineering, University of Leeds, Leeds UK

UNIVERSITY OF LEEDS

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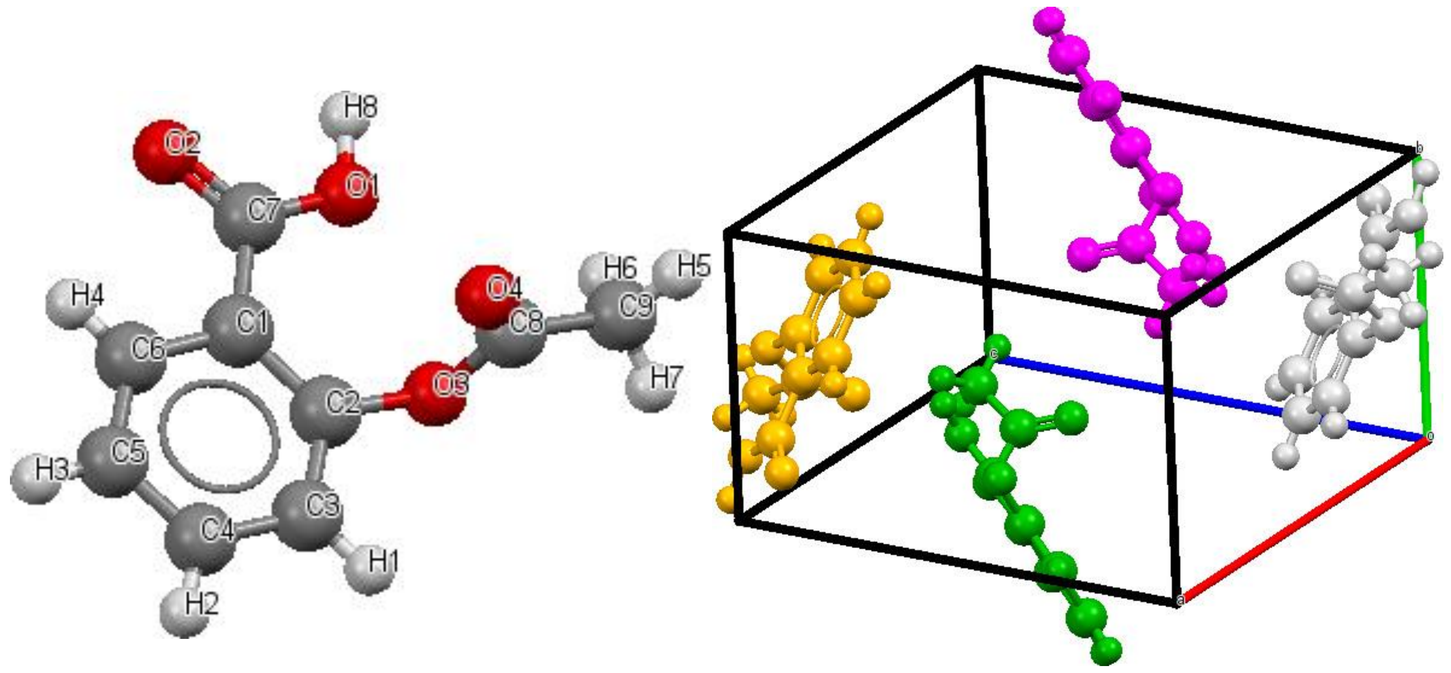
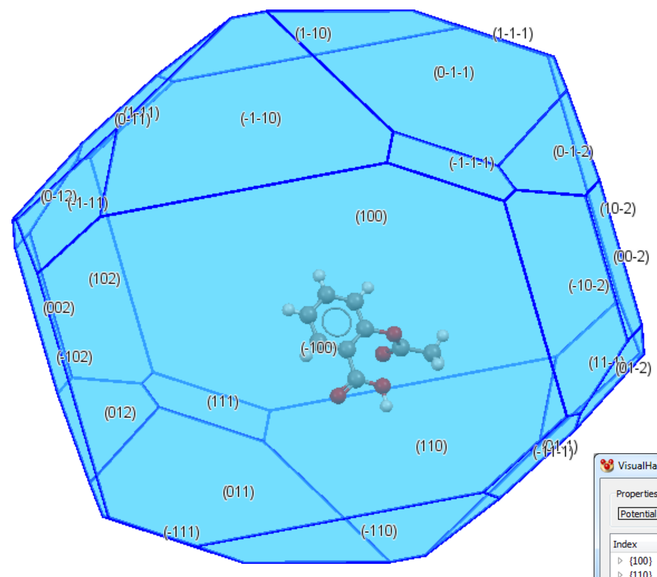
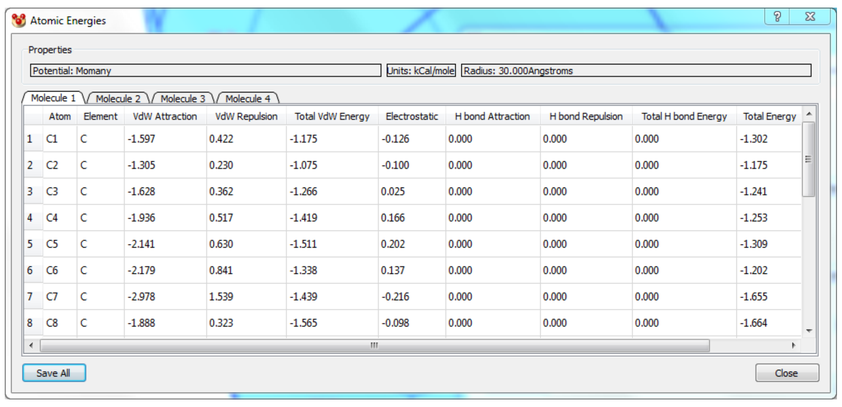
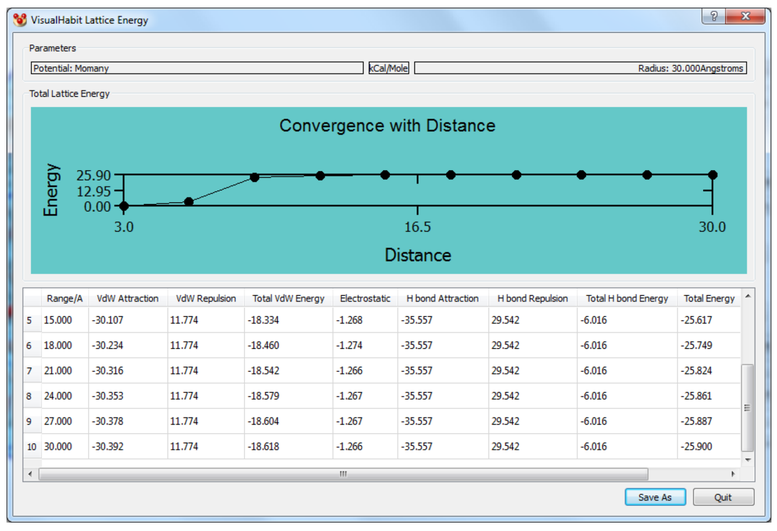
Molecular crystals are held together by a combination of forces: the London dispersive force between atoms; hydrogen bonding between specific functional groups; and electrostatic forces. Representing these forces with a potential function and using atom positions known from x-ray diffraction the properties of crystals can be predicted.

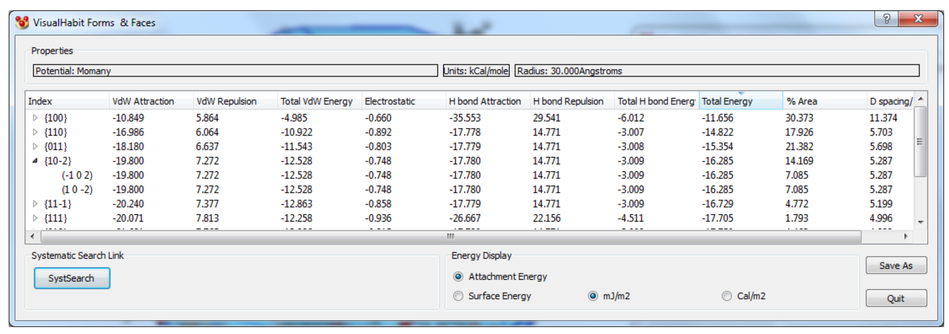
VisualHabit [1] is a software tool that, developed within CCDCs Materials Mercury [2] uses takes the crystallographic description of a crystal and converts it to a molecular representation onto which an atomistic potential can be applied. The crystallographic representation may not contain data on the atoms bonding. The molecular representation consists of one unit cell's worth of molecules, with the atoms properly bonded and possessing potential types and partial charges.

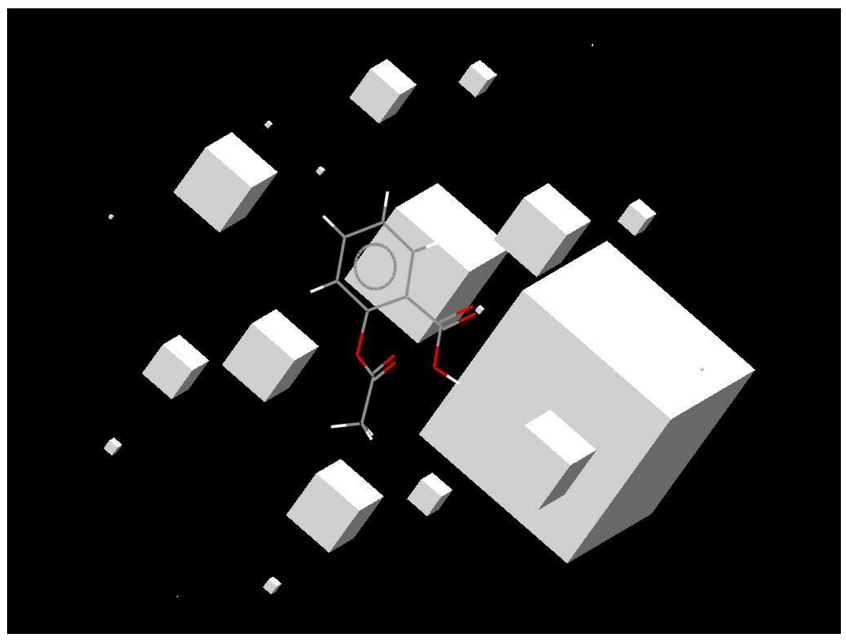


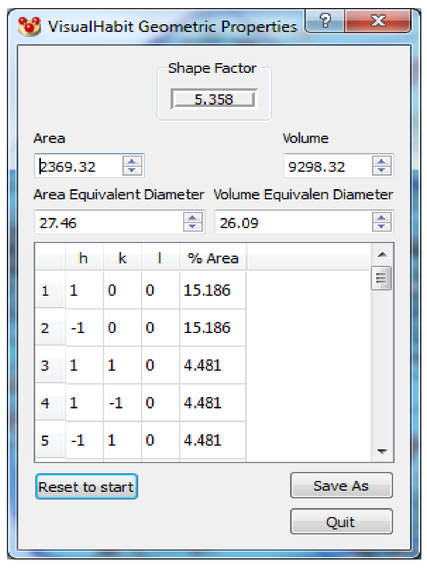












VisualHabit also uses the potential to calculate the lattice energy and use an attachment energy model is used to predict the crystal shape. Surface energies for the faces in the predicted shape can be calculated. The energies can be broken down by the types of interaction used in the potentials (van der Waals, hydrogen bonding and electrostatic).

1. Pickering JH, Hammond RB, Ramachandran V, Soufian M, Roberts KJ (2017) Synthonic Engineering Modelling Tools for Product and Process Design, Chapter 1 in Engineering Crystallography: From Molecule to Crystal to Functional Form (Editors: Roberts KJ, Docherty R and Tamura R), Springer Advanced Study Institute (ASI) Series, 2017, in press
2. C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward, The Cambridge Structural Database, Acta Cryst. (2016). B72, 171-179, DOI: 10.1107/S2052520616003954

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