## VisualHabit: Molecular Modelling of Crystals





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 developed within that, 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.



(012)

(011)

Ate	Atomic Energies													
Pro	Properties													
Po	Potential: Momany Units: kCal/mole Radius: 30.000Angstroms													
Mo	Molecule 2 Molecule 3 Molecule 4													
	Atom	Element	VdW Attraction	VdW Repulsion	Total VdW Energy	Electrostatic	H bond Attraction	H bond Repulsion	Total H bond Energy	Total Energy	<u> </u>			
1	C1	с	-1.597	0.422	-1.175	-0.126	0.000	0.000	0.000	-1.302				
2	C2	С	-1.305	0.230	-1.075	-0.100	0.000	0.000	0.000	-1.175	E			
3	C3	С	-1.628	0.362	-1.266	0.025	0.000	0.000	0.000	-1.241				
4	C4	С	-1.936	0.517	-1.419	0.166	0.000	0.000	0.000	-1.253				
5	C5	С	-2.141	0.630	-1.511	0.202	0.000	0.000	0.000	-1.309				
6	C6	С	-2.179	0.841	-1.338	0.137	0.000	0.000	0.000	-1.202				
7	C7	С	-2.978	1.539	-1.439	-0.216	0.000	0.000	0.000	-1.655				
8	C8	С	-1.888	0.323	-1.565	-0.098	0.000	0.000	0.000	-1.664	-			
•										Þ				
S	Save All Close													

-	rms of races			_	200			_		L V	
Properties											
Potential: Moma	any				Units: kCal/mole Ra	I/mole Radius: 30.000Angstroms					
Index	VdW Attraction	VdW Repulsion	Total VdW Energy	Electrostatic	H bond Attraction	H bond Repulsion	Total H bond Energ	Total Energy	% Area	D space	
▷ {100}	-10.849	5.864	-4.985	-0.660	-35.553	29.541	-6.012	-11.656	30.373	11.374	
▷ {110}	-16.986	6.064	-10.922	-0.892	-17.778	14.771	-3.007	-14.822	17.926	5.703	
▷ {011}	-18.180	6.637	-11.543	-0.803	-17.779	14.771	-3.008	-15.354	21.382	5.698	
▲ {10-2}	-19.800	7.272	-12.528	-0.748	-17.780	14.771	-3.009	-16.285	14.169	5.287	
(-1 0 2)	-19.800	7.272	-12.528	-0.748	-17.780	14.771	-3.009	-16.285	7.085	5.287	
(1 0 -2)	-19.800	7.272	-12.528	-0.748	-17.780	14.771	-3.009	-16.285	7.085	5.287	
▷ {11-1}	-20.240	7.377	-12.863	-0.858	-17.779	14.771	-3.009	-16.729	4.772	5.199	
▶ (111)	-20.071	7.813	-12.258	-0.936	-26.667	22.156	-4.511	-17.705	1.793	4,996	

	_	3.0		16.5								
	Distance											
	Range/A	VdW Attraction	VdW Repulsion	Total VdW Energy	Electrostatic	H bond Attraction	H bond Repulsion	Total H bond Energy	Total Energy			
5	15.000	-30.107	11.774	-18.334	-1.268	-35.557	29.542	-6.016	-25.617			
6	18.000	-30.234	11.774	-18.460	-1.274	-35.557	29.542	-6.016	-25.749			
7	21.000	-30.316	11.774	-18.542	-1.266	-35.557	29.542	-6.016	-25.824			
8	24.000	-30.353	11.774	-18.579	-1.267	-35.557	29.542	-6.016	-25.861			
9	27.000	-30.378	11.774	-18.604	-1.267	-35.557	29.542	-6.016	-25.887			
10	30.000	-30.392	11.774	-18.618	-1.266	-35.557	29.542	-6.016	-25.900			
•												

VisualHabit Lattice Energy

Parameters

Potential: Momany

Total Lattice Energy



8	🖇 V	isuall	Habit	Geor	netric Pro	perties	୧	x				
				s	hape Facti 5.358	or I						
	Area	э			Volume							
	<u>236</u>	59.32	*			92	298.32	*				
	Area Equivalent Diameter Volume Equivalen Diameter											
	27.	46			<del>2</del> 6.0	09 🚔						
		h k l		% Area			^					
	1	1	0	0	15.186							
	2	-1	0	0	15.186							
	3	1	1	0	4.481							
	4	1	-1	0	4.481							
	5	-1	1	0	4.481			-				
	Res	set to	start				Save	As				
	Quit											

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

ADDoPT is a collaboration instigated by the Medicines Manufacturing Industry Partnership, and part funded under the Advanced Manufacturing Supply Chain Initiative, a BEIS initiative delivered by Finance Birmingham and Birmingham City Council.

