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Atomic Surface Modeling and AIM Charges

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The quantum theory of "Atoms in Molecules" (AIM)[1] is a powerful method to get a molecular partitioning having a physical meaning. The zero flux electron density gradient surfaces define the atomic sub-volumes within chemical systems. Therefore, intrinsic atomic properties like charges and electric moments can be estimated from a 3D integration over the atomic basins. Nowadays, several softwares are available for this purpose and are frequently used in theoretical or experimental topological electron density studies. However, the analytical representation of the atomic boundaries requires sophisticated interpolations and is computationally expensive. Recently, a fast and robust numerical algorithm based on the steepest-ascent method was proposed by Henkelman *et al*[2] for the computation of the AIM charges. In this method, every mesh point in the cube containing the studied molecule is assigned to the atom to which the corresponding electron density belongs to. Therefore, surfaces encompassing the atomic basins can be defined numerically as a cloud of points. Popelier was the first who proposes the calculation of the IAM charges by using the Gauss divergence theorem on the flux of the electric field.[3] However, particular interpolations were used in his method to delimitate the atomic boundaries which are defined analytically in spherical geometries. In the present work, the atomic surfaces are treated numerically from the Henkelman method[2] as a cloud of points. In order to calculate the flux of the electric field, these points are taken as vertices of Delaunay triangles and exact reconstructions of the atomic boundaries are carried out.[4] Advantages and generalizations of this new approach to small and larger molecules will be discussed.
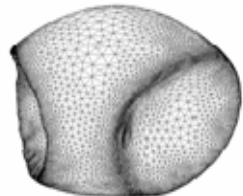
triangulated surface of the oxygen atom in water molecule

[1] R. F. W. Bader, *Atoms in Molecules: A Quantum Theory.* Oxford University Press, Oxford, 1990.
[2] E. Sanville, S. Kenny, R. Smith, G. Henkelman, *J. Comput. Chem.* 28 (2007) 899.
[3] P.L.A. Popelier, *Theor. Chem. Acc.* 105 (2001) 393.
[4] Gamma Project. INRIA, Rocquencourt, France.

MS14 P06

Can crystal structure prediction predict whether a salt or a cocrystal will be formed? Katarzyna E. Hejczyk,[a], Graeme M. Day,[a], William Jones,[a]; [a]*The Pfizer Institute for Pharmaceutical Materials Science, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK.* E-mail:keh49@cam.ac.uk

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An estimated about 75% of all drug molecules used in medicinal therapy are formulated as salts. The solid-state properties of a drug, as well as its properties in solution, can be modified by salt formation. Therefore, molecular modelling and successful structure prediction can open new opportunities, not only in the design of drugs but also in the study of their solid-state properties [1].
We are studying the contrasting crystallisation behaviour of some acids:base combinations in terms of salt or cocrystal formation. It has been reported by Haynes *et al*.[2] that succinic acid forms only cocrystals with the lutidines, while fumaric acid forms salts with some isomers, but cocrystals with others. We are investigating whether computational methods can explain whether a cocrystal or a salt will be formed when an acid and a base are combined and what factors determine the nature of the observed crystal structure.
Our study is based on comparison of energies (molecular and lattice) between the observed and corresponding hypothetical systems (cocrystals and salts). Crystal structure prediction calculations are presented for selected systems; these calculations successfully locate the observed structure in the vicinity of the lowest energy calculated structure.

[1] Handbook of Pharmaceutical Salts: Properties, Selection and Use, ed. P.H. Stahl and C. G. Wermuth, Wiley-VCH/VHCA, Weinheim/Zürich, 2002
[2] D. A. Haynes, W. Jones and W. D. S. Motherwell, *CrystEngComm*, (2006), 8, 830 – 840.

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Structure and Magnetism in Prussian Blue Analogues: Theory and Experiment. L. M. Lawton, D. S. Middlemiss and C. C. Wilson, *Department of Chemistry and WestCHEM Research School, University of Glasgow, UK*. E-mail: Lorrla@chem.gla.ac.uk

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The Prussian Blue Analogue (PBA) structure is a three-dimensional lattice of magnetic ions that interact via intermediate cyanide ligands. The structure directing property of these particular ligands and the flexibility of the structure allow ions of specific spin and oxidation states to be selected, so that the exchange interactions behave as predicted from fundamental orbital rules. The most important corollary of this fact is it has proved possible to synthesise PBAs with specific structure and properties, obtained primarily by inclusion of varying ratios of the magnetic ions, but also by application of external perturbations.
Ohkoshi and Hashimo [1] studied the saturation magnetisation as a function of x in the $\{Ni_x^{II} Mn_{x-1}^{II}\}_{1.5}$ $[Cr^{III}(CN)_6]$ •nH_2O family and at x~0.4 this was found to switch from antiferro-ferromagnetic ordering. Pressure