

devices and sensors, etc. In order to effectively control the processing, structure and performance of these nano-materials, there is a priority on the development of robust non-destructive techniques for imaging nano-particles. The destructive and generally two-dimensional nature of electron microscopy often limits the nano-particle imaging to qualitative or semi-quantitative analysis. X-ray small-angle scattering can estimate the average scale of nano-particles over a large area/volume without destroying the specimen, however it does not resolve the shape of the particles. Here we show that x-ray diffraction intensity collected as a multi-dimensional function of scattering angle can be treated to reconstruct the three-dimensional (3D) shape of an average nano-particle with a spatial resolution of a few nanometres.

Our results demonstrate that this approach to x-ray diffraction data analysis provides the potential for 3D non-destructive analysis [1]. The methodology is based on the measurement of a high angular resolution x-ray Fraunhofer diffraction patterns with further application of a phase-retrieval formalism. The advantage of experimental data collection in momentum transfer (angular) space is that the diffraction pattern of the object is not susceptible to any of its linear translation and, consequently, the intensity distribution measured as a function of the angular direction in reciprocal space does not require coherent radiation and/or extraordinary stability of the radiation source and/or sample. The non-destructive nature of the technique renders it perfect for *in-situ* studies of nucleation and growth of nanoparticles in engineered nanocomposites [2]. The possibility of using incoherent x-ray sources allows the method to be implemented in any laboratory [1]. The only principal restriction on achievable resolution is the physical limit of the order of sub-nanometer.

We present results relative to ~50 nm diameter nano-particles dispersed in a polymer matrix with a spatial resolution of 2 nm, 50-350 nm intermetallic nanoparticles in ultra-strong Al-Cu alloys with a spatial resolution of 5-8 nm, and ~10 nm diameter carbon nanotubes with spatial resolution of 1 nm. Unlike a microscopy technique, the method to be presented does not allow one to distinguish the shape and size of individual nanoparticles within a distribution. This limits the application of the method to studies of structures with mono-dispersed nanoparticles. However, this very same limitation is a significant advantage of the method for materials science as it does allow non-destructive, *in-situ* analysis over large volumes (several mm³) of material, with determination of the modal shape-size of the dispersed particles and a close evaluation of the distribution of particle sizes [3].

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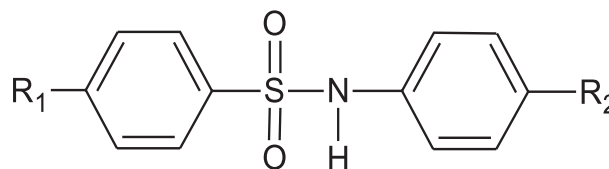
Can heats of sublimation and melting points of organic crystals be predicted?

John Kendrick,^a Frank J.J. Leusen,^a Michael B. Hursthouse,^b Yuanxin Ding,^b ^a*School of Life Sciences, University of Bradford, Bradford, BD7 1DP, (UK)*. ^b*School of Chemistry, University of Southampton, Southampton, SO17 1BJ, (UK)*. E-mail: j.kendrick@bradford.ac.uk

The accurate calculation of the lattice energies of small organic molecules has only recently become possible as a result of developments in Density Functional Theory (DFT), including the introduction of several methods for the incorporation of non-local dispersive interactions. Much has been done to verify these developments using very accurate molecular calculations, but few publications address the validity of these methodologies for organic molecular crystals [1]. The

experimental heats of sublimation of 33 compounds will be compared with the lattice energy predictions of some of the latest solid state DFT methods. In particular, methods incorporating a dispersive correction through a damped molecular mechanics type interaction [2] (DFT(D)), will be compared with new approaches incorporating dispersive interactions as part of the functional [3]. A method incorporating dispersion as part of the functional will be shown to perform slightly better than the best DFT(D) method.

The possible prediction of melting point from knowledge of molecular structure alone has intriguing possibilities and many quantitative structure property relationships (QSPRs) [4] have been developed to allow the prediction of melting point with varying degrees of success. There is a rule of thumb that relates trends in melting points to lattice energies and, using one of the solid state DFT methods used in the study of heats of sublimation, accurate lattice energy calculations are performed on a series of 4,4'-disubstituted benzenesulfonamidobenzenes. Experimental crystal structures and melting points are available for 100 compounds with the generic molecular structure shown in the Figure. [5]. The substituents considered include Br, CF₃, Me, Cl, CN, F, H, I, NO₂ and MeO. Solid state DFT calculations are used to optimise the geometry and unit cell of all the observed crystal structures. A comparison of the deviations between the experimental and calculated geometries allows the accuracy of the geometrical predictions of the method to be assessed. The minimised lattice energies are then used to establish correlations with the observed melting points. Preliminary results indicate that there is a significant correlation for an isostructural subset of the molecules.



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An entire class of new compounds forming polar crystals

Roberto Centore,^a Mojca Jazbinsek,^b ^a*Department of Chemistry "Paolo Corradini", University of Naples "Federico II", I-80126 Naples*. ^b*Nonlinear Optics Laboratory, ETH Zurich, CH-8093 Zürich*. E-mail: roberto.centore@unina.it

In a polar crystal there is a direction which is not transformed in the opposite direction by any symmetry operation of the crystal class; that direction is the polar axis of the crystal. Centrosymmetric crystals are not polar, because the center of symmetry transforms any direction in the opposite one. However, only 10, out of the 21 crystal classes lacking the center of symmetry, are polar. In spite of their rarity, polar structures are very interesting. In fact, several functional properties requested in materials for advanced applications (piezoelectricity, pyroelectricity, ferroelectricity, second harmonic generation, electrooptic response) are only allowed or they are enhanced in polar structures.

Many strategies used for increasing the probability of getting a polar crystal are based on overriding dipole-dipole interactions and include