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Keywords: XAFS, time-resolved studies, spin

P02.10.16

Indexing algorithm for powder diffraction pattern using topograph

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Indexing of powder diffraction patterns is considered as the most difficult part among the procedures of ab-initio powder structure determination. Recently, we devised a new indexing algorithm that can search rapidly and thoroughly for the possible solutions. Topograph is a connected tree in the graph theory, which is a collection of relation formula given by $Q(h1+h2) + Q(h1-h2) = 2 * (Q(h1) + Q(h2))$. Although this formula is already known as Ito's equation and used in Ito's algorithm, it takes a more powerful role in our method as a basis of the equations among the Q-values of the peaks. Extinction rule is troublesome, but it is somehow obtained without information on the symmetry, in the process to construct the topograph. The algorithm is proved to work completely at least for lattices of dimension 2. For the case of dimension 3, some uncertain part still remains. The algorithm works without any assumption on Bravais lattice. It is efficient even if there is a false peak in the powder diffraction pattern or the material is not a single phase. The detail of the method and some results are introduced.

Keywords: powder indexing, *ab-initio powder* structure determination, computer algorithms

P02.10.17

Structural characterization and developing a suitable SAXS model of diblock(DEAEMAn-DMAEMAm) polymers

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Small Angle X-ray Scattering (SAXS) is a powerful method to investigate nano-aggregations formed by self-assembly of block copolymers in melt, solution or crystal state [1]. In this study, theoretical scattering models such as spherical core-shell and ellipsoidal core shell micelle models were described and discussed after the performed SAXS measurements at NSRRC-Taiwan beside the determination of the morphologies. The studied di-block copolymers [2-(diethylamino)etyhyl methacrylate (DEAEMAn)]・[2-(dimethylamino) etyhyl methacrylate (DMAEMAm)] had been synthesized by Vural Bütün as a part of a serial research on pH dependent-water soluble block copolymers [2-3]. Our previous studies have been showed that micellar aggregations are expected due to hydrophobic and polyelectrolyte ends of polymeric units [4]. Two samples which have 23576 and 12177 g/mol molecular weights were prepared for SAXS measurements. Model-independent approximations with Guinier, Porod and Kratky plots together with the results of static and dynamic light scattering (SLS and DLS) are used to extract morphology characteristics, on which basis, a suitable model shape is chosen to fit the SAXS profiles. Beside of these investigations, a semi-empirical calculation method (PM3 [5]) was also used to examine crosslink effect of free polymeric units. So, electron densities in the layered thicknesses were also predicted before construction of the models. At the end of the study, the details related with mathematical and physical explanation for the models are also described in this presentation.

Keywords: DEA, DMA, Core-shell, SAXS, DLS, SLS, PM3, Nano structures

P02.10.18

High-pressure phase transformations in aragonite, strontianite and witherite

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We have studied structural phase transformation in aragonite $CaCO_3$ and related isostructural compounds strontianite $SrCO_3$ and witherite $BaCO_3$ at high pressure by performing first principle calculations. The following phase transition sequence *Pmmn - Pmcn - C*222$_1$ have been found for all three compounds. Furthermore, $CaCO_3$ and $SrCO_3$ undergo a phase transition from *C*222$_1$ to Pmmn modified-aragonite phase at very high pressure as a result of carbon sp^2 to sp^3 transition. Thus the structural trends of these compounds are determined by both the cation size and the chemistry of CO_3 group. The formation of sp^3 hybridized bonds is driven by the intrinsic property of the carbon atom to form tetrahedrally covalent bonds at high pressure and explains the stability of $MgCO_3$ and $CaCO_3$ at the Earth's lower mantle pressure conditions. The presence of sp^3 hybridized carbon may serve as a criterion for new possible high-pressure phases of carbon bearing minerals.

Keywords: *ab-initio* calculations, high-pressure phase transformations, carbonates

P02.10.19

Crystal structures of moderately complex organic molecules are predictable

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P2

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A comprehensive computational strategy for the prediction of crystal structures is presented that has scored an unprecedented 4 in 4 success rate at the 2007 CCDC blind test on crystal structure prediction [1]. Key components of the new approach, implemented in the GRACE software package, are a hybrid method for the accurate calculation of lattice energies, a robust procedure for the parameterization of tailor-made force fields and a novel approach for crystal structure generation. The hybrid method combines DFT calculations by means of the VASP program with an empirical van der Waals correction. It is used for the final lattice energy ranking and acts as a reference standard for force field parameterization. A tailor-made force field is derived for each molecule to be considered and used for crystal structure generation as well as for the preparation of second derivative matrices for the final lattice energy optimization with the hybrid method. Based on the known statistical deviation between the tailor-made force field and the hybrid method, a shortlist of crystal structures from a small energy window is selected for the final lattice energy optimization and ranking. In addition to the blind test results, validation studies for 15 organic molecules are presented, including ethane, ethylene, acetylene, methanol, urea, acetic acid, cyclohexane-1,4-dione, paracetamol, CCDC blind test molecules I to VI and a pharmaceutical compound for which crystal structures have been predicted in a blind test fashion. 17 out of the 18 experimentally observed crystal forms of these molecules are found among the first two most stable predicted crystal structures.

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Keywords: crystal structure prediction, computer modelling solids, polymorphism

P02.10.20

Structure prediction of flexible small molecules - A case study

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Predicting the crystal structures of small molecules from energy calculations is of considerable interest for a number of scientific and industrial purposes. However, in the field of polymorph-forming pharmaceuticals two main problems arise. One is the high degree of internal flexibility of many of the molecules of interest and the consequential large number of possible conformations. The resulting multitude of packing possibilities can overwhelm even fast computers. The other problem is that many of these structures have similar energies. Exact energy modeling is thus necessary to identify the real structures. We checked possible strategies using aripripazole as a test case. For this compound, a number of polymorphs and various solvates are known, as are their respective crystal structures. By comparing the experimental structures with the calculations on all stages, a number of helpful results were established: 1) Quantum-mechanical (QM) energy calculations on the isolated molecule reduce the number of possible conformations drastically. For aripripazole, seven torsional degrees of freedom allow 2916 minimum conformations. Of these, only 296 remain, once correlation of neighboring torsions is considered. Further reduction is possible, if the influence of hydrogen bonds is considered. 2) The molecule

has five potential hydrogen bond acceptor sites, but QM calculations reveal that only one of these is realizable. The corresponding hydrogen bonds are realized in all experimental structures. 3) The experimental structures account for all the lowest energies found. Thus, any problem in finding the correct structures is not due to the energy model, but is a matter of the search algorithm and processor time. The treatment of the hydrogen bonds was found to be crucial in this.

Keywords: structural prediction, pharmaceutical organic molecules, energy calculations

P02.10.21

Increasing the effectiveness of evolutionary crystal structure prediction using fingerprint-function

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Evolutionary algorithm approach to crystal structure prediction problems has proven its effectiveness in various applications. Algorithm USPEX (Universal Structure Predictor: Evolutionary Xtallography) allows one to predict the most stable crystal structure for a given compound without requiring any experimental input. This is especially attractive for simulation of materials under extreme conditions. However, the inability to determine the degree of similarity between different structures limits the effectiveness of the algorithm and increases the probability of trapping in a particular basin of the energy surface. To solve this problem we derived a family of specially constructed fingerprint-functions. Fingerprint-function is a function, that is independent of lattice vectors choice and uniquely determines the structure of the crystal. Another important property of these functions is that the degree of correlation between functions calculated for two structures can be used as a good measure for degree of similarity between those structures. We have shown, that after modifying selection and variation operators with the help of fingerprint-functions, the effectiveness of USPEX algorithm was increased. This method also simplifies the search for metastable states by evolutionary algorithms.

Keywords: crystal structure prediction, *ab-initio structure* determination, computer algorithms

P02.10.22

Inverse multislice calculations: A new method for solving complex structures

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The multislice approach has been used for 50 years to find the result of a wave passing through a thick sample. One problem with multislice is that it is difficult to reverse the calculation and find the structure of a sample given measurements of the exit wave. This limits the use of multislice techniques in experimental microscopy, as in general the sample structure is unknown and the aim is to find it. Iterative algorithms for microscopy have been studied since the