

1970s. In recent years significant results have been achieved with their use. However iterative algorithms to date can only retrieve the complex transmission function of a thin sample. Thicker samples, where dynamical diffraction and propagation are important, can not be examined with these techniques. A recent innovation combines theptychographical iterative engine technique of phase retrieval, with the multislice method. The result is an iterative approach that uses measured intensities of the exit wave to find the transmission functions of the slices that represent the sample structure. This generalisation of the iterative technique allows the retrieval of depth information in the sample. Much thicker structures can be analysed than was previously possible with such approaches. It is potentially possible to use the technique to solve a structure that is periodic or aperiodic in any direction. The technique is experimentally simple, requiring only a series of intensities recorded at different positions of the incident beam plus known information about that beam. The applications of this approach include any experimental situation where intensities can be measured and a thick, periodic or aperiodic sample is analysed. This includes a huge number of possibilities in crystallography and many other fields.

Keywords: inverse problem, computational methods, structure determination

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Rapid and routine determination of hydrogen positions in inorganic and organometallic compounds

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Hydrogen is a fundamentally important element in many key areas of inorganic materials design, including development of technological materials (e.g. hydrogen storage media and proton-conductor fuel cell components), functional framework materials (e.g. zeolites), catalysts, organometallic co-ordination complexes and inorganic hydrates. Due to weak X-ray scattering by light elements, and hydrogen's large incoherent neutron background, determination of hydrogen positions in inorganic materials traditionally necessitates costly sample deuteration or painstaking synthesis of large single crystals for neutron diffraction. This limitation is now being addressed via development of experimental and data refinement methodologies utilising high flux neutron powder diffractometers such as D20 at ILL. We present a selection of results demonstrating application of this new methodology to technologically important inorganic material systems with significant hydrogen content. These include in-situ studies of functional zeolites (e.g. industrial catalysts ZSM-5 and mordenite, having adsorbed hydrogenous molecules) and metal ammoniates such as Ni(NH₃)₆Cl₂ (candidate hydrogen storage materials). Further examples include organometallic compounds such as Zeise's salt and complexes requiring exact determination of hydrogen position (e.g. those with potential agostic hydrogens). The full structures of some heavy metal salt hydrates are also presented, confirming that hydrogen positions can be accurately determined alongside metals as heavy as uranium and bismuth. As well as highlighting the applicability and potential impact of these new methods, this work is aimed at establishing these methodologies as a valuable tool for routine study of hydrogenous materials across all inorganic fields.

Keywords: characterization methods, hydrogen, neutron and X-ray diffractometry

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Development of polarizable force field for the prediction of molecular crystal structures

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Prediction of crystal structures for organic molecules has great importance in many industries like pharmaceuticals, pigments, dyes, and so forth, because many of the macroscopic properties of their products are highly dependent on their crystal structures. The accuracies of predictions for lattice constants and molecular geometries in crystal depend on the performance of intermolecular potential which is normally described as the electrostatic and van der Waals terms in empirical force fields. Although electrostatic parameters of partial atomic charges are generally unchanged in a potential energy calculation during geometry optimization and dynamics simulation, the charge distribution of a molecule should vary depending on conformational transformations and induced interactions with other molecules. To estimate the charge distribution according to their changes, the charge equilibration (QEq) approach [1] is proposed and can provide appropriate partial atomic charges for sufficient representation of the electrostatic interactions. Recently, we proposed new framework of QEq, named NQEq [2], that the empirical formula of Coulomb interaction is employed and that the parameter set is divided into each atom types based on Merck Molecular Force Field (MMFF) [3]. In this presentation, we introduce our extension of NQEq to molecular crystal calculations. This attempt can be obtained the appropriate charge distributions polarized by periodic environment. We will also show the results of lattice constants optimization for some organic molecular crystals using its NQEq and MMFF.

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Drug virtual screen by GA/GP: Docking studies with tubulin inhibitors as anticancer agents

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It is expected to shorten the required research time spent in the early stage of development of drug design through computer calculation. Computer Aided Drug Design is one of the most powerful concepts applied to satisfy such demand. Upon docking simulations, it is allowed to find out the binding sites and orientations between target