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COMPUTER PREDICTIONS OF ORGANIC CRYSTAL STRUCTURES AND PROPERTIES

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How do intermolecular forces determine the crystal structure adopted by an organic molecule? The challenge of predicting the quantitative crystal structure from the chemical diagram of a molecule requires reliable quantitative models for the intermolecular forces. We have been deriving anisotropic atom-atom model potentials from the *ab initio* molecular charge density, which automatically represent the effects of lone pair and π electron density on the intermolecular interactions. These have proved necessary to compare the relative thermodynamic stability of different hypothetical structures as the first stage in crystal structure prediction. However, often many more energetically feasible structures are predicted than known polymorphs. Thus, the second challenge is to model how these forces determine the kinetic factors that can affect the polymorph obtained [1]. The computed mechanical and morphological properties of the hypothetical structures can be used [2] as a starting point to eliminate kinetically improbable structures. Computer crystal structure predictions are at an exciting stage for simple organic molecules. There have been many successes, including in blind tests [3]. However, even after eliminating structures on the basis of both energy and properties, we are often predicting more potential polymorphs than had been observed. Such predictions are leading to the discovery of new polymorphs. These early examples show that considerable experimental and theoretical collaboration is required for a predictive understanding of polymorphism.

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THE NON-CRYSTALLOGRAPHIC PHASE PROBLEM AND OPPORTUNITIES WITH FREE ELECTRON LASERS

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The X-ray Free Electron Laser (FEL) is an accelerator based device that offers the promise of a high intensity beam consisting of very short pulses (eg. 230 fsec for the Linac Coherent Light Source proposed at Stanford) of almost fully coherent x-rays. The beam will have a brightness one or two orders of magnitude greater than that of a modern synchrotron. FEL devices will be providing beams in the next decade or so and it is important to identify the best science that can be done with them.

The intensity of the light in the FEL beam will destroy many samples and so the results of the experiment will often rely on the extraction of information scattered by the sample as it disintegrates. The key challenge, then, is to extract the maximum possible information from the radiation scattered by arbitrary (that is, non-crystallographic) samples. Clearly complete information will require the ability to extract both the amplitude and the phase. Recent work has made considerable progress in developing methods for the extraction of phase information from radiation scattered by such samples. Some approaches are based on extensions of the Gerchberg-Saxton algorithm, and others on measurements at different physical locations. Excellent results have been obtained with the latter approach for visible light, electrons, neutrons and x-rays.

In this talk I will review the progress made in solving the non-crystallographic phase problem and place these developments in the context of the prospects offered by an FEL.

Keywords: PHASE PROBLEM; FREE ELECTRON LASER; NON CRYSTALLOGRAPHIC

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MATERIALS DESIGN

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One of the most challenging tasks in inorganic materials science is the design of new materials with previously defined physical or chemical properties. To reach this objective two different approaches are, in general, explored: 1. The first approach is to simulate the motion of the atoms in the material, as well as their electronic interactions, as close to reality as possible by using quantum-mechanical calculations. 2. The second approach is based on a more pragmatic level and consists in searching for patterns and rules in experimental results published in the literature. We focus here mainly on the second approach. There exist a relatively large amount of published data for binaries, much less for ternaries and almost no data for multinaries. Therefore, the most efficient way to go is to search for regularities, such as laws, rules, principles, factors, tendencies, and patterns, among binaries and then to try to extend them to multinaries. for materials design we intend to reduce materials properties (e.g. crystal structure, physical properties, etc.) to expressions of atomic properties of the constituent chemical elements. The relations are very complex, but the much regularity published in the literature proves that they are not only of a qualitative nature but in many cases also quantitative. The success of 'data-driven' computational inorganic materials design depends on the availability of experimental data of appropriate quality, if possible organized in one large phase-oriented database. With this purpose the PAULING FILE* project was started in 1995.

* for information see www.paulingfile.com

Keywords: INORGANIC MATERIALS DESIGN, STRUCTURE-PROPERTY RELATIONSHIP, DATABASES

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PRESSURE, LIFE AND MOLECULES

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Proteins can be denatured/unfolded by high hydrostatic pressure and this gives rise to an elliptic stability phase diagram in the temperature-pressure plane. The observation that stability diagrams for bacteria, viruses and other complex systems are similar to those obtained for proteins suggests that proteins are the primary target in the pressure and temperature behavior of organisms. One of the interesting differences between the pressure- and temperature-induced unfolding is that in many cases the temperature-unfolded protein has a strong tendency to form intermolecular aggregates. Because of its important role in a number of diseases, the mechanism of the formation of aggregates deserves closer attention. Pressure- as well as temperature-induced effects are closely connected with the presence of water. However, pressure-induced amorphization has been observed in inorganic substances, liquid crystals, synthetic polymers and starch. This gives some new directions for the interpretation of the observed effects in water-soluble biopolymers. Pressure, as well as temperature, causes changes in the interaction of the biopolymer with the solvent (hydration) but the imperfect packing effects in the interior (cavities) also contribute to the re-entrant behavior of aqueous solutions of proteins and starch. A good overview of these and other aspects are discussed in contributions to a special issue of Biochimica Biophysica Acta on 'Frontiers in High Pressure Biochemistry and Biophysics.

Keywords: HIGH PRESSURE, BIOMOLECULES