random phason is taken into account as the phason displacement parameter in the refinement. The paper demonstrates structure determination of quasicrystals in the light of recently developed techiniques.

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Keywords: quasicrystals, structure refinement, direct methods

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Structure of Protein Assemblies by Comparative Modeling and Electron Microscopy

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We explore structural characterization of protein assemblies by a combination of electron cryo-microscopy (cryoEM) and comparative protein structure modeling (1). Specifically, our method finds an optimal atomic model of a given assembly subunit and its position within an assembly by fitting alternative comparative models into a cryoEM map. The alternative models are calculated by MODELLER (2) from different sequence alignments between the modeled protein and its template structures. The fitting of these models into a cryoEM density map is performed by a new density fitting module of MODELLER (Mod-EM). Identification of the most accurate model is based on the correlation between the model accuracy and the quality of fit into the cryoEM density map. To quantify this correlation, we created a benchmark consisting of eight proteins of different structural folds with corresponding density maps simulated at five resolutions from 5 to 15 Å, with three noise levels each. Each of the proteins in the set was modeled based on 300 different alignments to their remotely related templates (12-32% sequence identity), spanning the range from entirely inaccurate to essentially accurate alignments. The benchmark revealed that one of the most accurate models can usually be identified by the quality of its fit into the cryoEM density map, even for noisy maps at 15 Å resolution. Therefore, a cryoEM density map can be helpful in improving the accuracy of a comparative model. Moreover, a pseudo-atomic model of a component in an assembly may be built better with comparative models of the native subunit sequences than with experimentally determined structures of their homologs.

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Keywords: comparative modeling, electron cryo-microscopy, fitting

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Quantum Mechanical Simulation of the Vibrational Properties of Garnets

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Structural, vibrational and electronic properties of pyrope, grossular and andradite have been simulated with the periodic *ab initio* CRYSTAL [1] program, that adopts a local variational basis set ("Atomic Orbitals") to build the crystalline orbitals. An *all-electron* basis and the B3LYP hamiltonian have been used.

The full spectrum at the Γ point (97 frequencies) [2] and the IR intensities have been evaluated, along with the symmetry of the modes, which is automatically determined. The eigenvectors of the dynamical matrix have been analyzed with different tools, including direct inspection, isotopic substitution, animations; classification-interpretation questions raised by previous studies are discussed.

The 17 IR and 25 RAMAN active modes are compared with available experimental data [3], [4]. The agreement is excellent in most of the cases (6-8 cm^{-1} the mean absolute difference).

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Keywords: ab-initio calculations, garnets, vibrational frequencies

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***In Situ* X-ray Study of Hydrothermally Prepared Titanates and Silicotitanates**

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In a typical ex-situ hydrothermal or solvothermal reaction the investigator knows what is input and what the end result is but has no experimental evidence of what transpires in between. In situ methods, whether using X-ray, NMR, IR or other techniques aims to follow the reaction through this in-between stage. For crystal growth studies, in-situ X-ray diffraction is eminently satisfactory. We will describe our crystal growth studies of titanium silicate phases and the ion exchange mechanism of Cs^+ ion uptake in their tunnel structures.

One of the most vexing problems facing the nuclear industry and countries with nuclear weapons is the safe disposal of the generated nuclear waste. Huge quantities of nuclear waste arising from weapons manufacture are stored at the Hanford and Savannah River sites. The general method of remediation involves the removal of Cs-137, Sr-90 and actinides from a huge quantity of salts, principally $NaNO_3$, organics and complexing agents. It has been found that a sodium silicotitanate is able to remove Cs^+ selectively from the waste and certain sodium titanates remove Sr^{2+} and actinides. These compounds have been prepared by ex-situ hydrothermal methods. We have studied the in situ growth of these materials at the National Synchrotron Light Source, Brookhaven National Laboratory.* In addition we will describe the mechanism of ion exchange in the titanosilicate as observed by in situ methods and how the combination of these techniques coupled with an intimate knowledge of the structure of the solids is helping to solve the remediation process. In general, the in situ method allows the investigator to follow the nucleation and crystal growth or phase transformations occurring in hydrothermal reactions, and as a result of ion exchange reactions.

* In collaboration with Aaron J. Celestian, Department of Geosciences and John B. Parise and Jonathan Hanson, Department of Chemistry, SUNY Stony Brook, NY, USA.

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Catalysts of *De Novo* Disulfide Bond Formation

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Disulfide bonds are crucial for the folding and stability of many cell-surface and secreted proteins. In addition, disulfides can be used for redox control of protein activity. *De novo* disulfide bond formation by enzymes such as those that drive oxidative protein folding requires transfer of electrons from dithiols to non-thiol electron acceptors. We have determined the structures of representatives of the two known eukaryotic enzyme families that catalyze this process. These enzymes, Ero1 and Erv2, are flavoproteins that share similar structural and mechanistic features despite a lack of sequence similarity. In particular, our crystallographic and enzymological studies suggest that both enzymes operate by a "disulfide shuttle" mechanism, in which a dithiol motif on a mobile segment of each enzyme transfers electrons from cysteines in substrate proteins to the rigid active-site disulfide. In