

# Oral Contributions

## [MS13-02] Combining Ab-initio Lattice Dynamics and Diffraction Measurements in Charge Density Studies

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The use of synchrotron radiation and large area detectors have helped with measurement of charge densities so that the quality and quantity of data has become much better within the last decade. These advances call for new and better models to interpret the data. New approaches to model the static charge densities have been proposed, many of which relying on high-level *ab-initio* calculations, either by direct refinement or by inclusion in libraries describing typical bonding situations [1-5]. Modeling of thermal motion in crystals has not received the same attention, yet the static densities and thermal motion are equally important: Together they conform the entire model refined against a single set of measured data. There is no doubt that a correct description of the thermal motion is crucial in order to obtain reliable estimates of the static densities [6,7]. We describe some new approaches to model atomic motion in crystals. The SHADE (Simple Hydrogen Anisotropic Displacement Estimator, <http://shade.ki.ku.dk>) approach to estimate H atom motion has proven to be useful for many systems, yet there are special bonding systems that require other approaches. We present an approach based on combining (segmented) rigid body refinement and periodic *ab-initio* calculations, and compare with previous approaches and neutron diffraction results. We also demonstrate the transfer of mean square displacements from one structure to another. Both approaches are implemented in a new update of the SHADE server [8]. Using information from periodic *ab-initio* calculations can be used to describe the vibration of not only hydrogen, but

also heavier atoms in the crystal. Our recent calculations of Debye-Waller factors for various test systems [9] has prepared the ground for proposing the refinement of normal modes of vibration against diffraction experiments. This last procedure opens the doors for refining data collected at multiple temperatures, as well as for modeling of thermal diffuse scattering.

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