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Fast Method for the Prediction of Intercrystalline Water Molecule Orientation in Ionic Crystals SEYEDAYAT GHAZISAEED, BORIS KIEFER, New Mexico State University — Water has previously been reported to affect electronic properties especially of molecules in solution. Thus, water in crystalline materials may be suitable for affecting the physical and chemical properties of the host material as well. However, the crystallographic description of hydrogen in crystalline materials is challenging since it scatters x-ray's poorly and neutron diffraction experiments require significantly larger samples. Therefore in many cases, the location of the hydrogen atoms remains unknown and cannot be obtained directly from crystallographic databases. Here we present a mathematically robust method for the prediction of hydrogen positions of intercrystalline water inside ionic inorganic crystals. We will show that the net torque provides a fast and simple method to establish the orientation of water molecules that avoids the conditional convergence problem of coulomb sums in ionic crystals. We will present and discuss the results of this method for several test materials and compare to available neutron data and *ab-initio* calculations. The successful determination of water molecule orientation is a necessary first step to address the question if and under what circumstances intercrystalline water can provide host materials with new functionalities.

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