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TORQUE, a Software Package to Predict Water Orientations in Ionic Crystals. SEYEDAYAT GHAZISAEED, BORIS KIEFER, New Mexico State Unive — It is well known that H2O can affect phase stability and materials performance. For example, water content in air can affect efficiencies of organic-inorganic perovskite solar cell. Thus, the experimental identification of water orientations is highly desirable but remains challenging due to the small scattering cross section of hydrogen. Similarly, first-principles computations depend strongly on unit cell size and available computing resources. We have developed a Linux based software package based on rotational equilibrium and point charge electrostatics for predicting the orientation of crystallization water molecules in ionic crystals. This method is at least ˜300 times faster than first-principles density-functional-theory (DFT) computations and provides optimized orientations that are consistent with experiment and theory. Interestingly, it provides a new H2O orientation in Kernite crystal that has not been reported previously. Our DFT computations show that the two conformations are energetically in-equivalent. Thus, the torque method provides a new, simple, robust, and fast method to complete initial structures for ab-initio computations of ionic materials that contain crystallization water and provide initial water orientations for experimental structure refinements.

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