The short range order in liquid water and amorphous ice

Neta Nir
Advisor: Prof. Guy Makov

Water is probably the most unique material on the planet in all states of matter: solid (ice), liquid (water) and gas (steam). It exhibits multiple anomalous properties, which are due to its intermolecular hydrogen bonding. In a liquid or an amorphous system, in order to determine the Short Range Order (SRO) it has to be described in a relatively simple way by a theoretical model.

The SRO in water and ice was determined from measured partial radial distribution functions (RDFs) by applying the Quasi Crystalline Model (QCM). Experimentally determined partial RDFs of water at various temperatures and pressures were considered, together with crystalline ice at 220K at ambient pressure as well as the three known phases of amorphous ice: Low Density (LDA), High Density (HDA), and Very High Density (VHDA). It was found that at low temperatures and pressures the SRO of water is similar to that of the ice Ih structure. At higher pressures and low temperatures the SRO of water becomes similar to that of tetragonal ice III structures with c/a ratio of 0.8. At higher temperatures of 573K the SRO obtained was similar to that of rhombohedral ice II. As for the amorphous ices, we conclude from the QCM analysis that these three forms are structurally distinct with SRO similar to those of ice Ih, ice III and ice II for the LDA, HDA, and VHDA respectively.
Exploring electronic properties of SnS cubic phase

Olga Korchev Khina

Advisors: Dr. Iris Visoly-Fisher and Prof. Yuval Golan

SnS is an earth abundant semiconductor with orthorhombic crystallographic structure that possesses attractive properties for photovoltaic and photocatalytic applications for renewable energy production, including near-optimal direct band-gap of 1.3eV, high absorption coefficient and high density of charge carriers. Recently, a new cubic binary phase of SnS was discovered in our group – a crystallographic structure of this material that was hitherto unknown. Preliminary research demonstrated unique properties, including increased band gap of 1.5-1.7eV, mechanical stability and p-type conductivity of the cubic SnS phase. In the current work, we aimed to characterize the electronic properties, i.e., $E_{\text{VH}}, E_{\text{C}}$ and $E_{\text{F}}$ of the cubic SnS phase and to compare them to those of its orthorhombic counterpart. To that end, we first synthesized thin films of cubic SnS phase using the chemical solution deposition method, which is an inexpensive, simple and environment-friendly growth technique. Subsequently, we performed contact potential difference and ultraviolet photoelectron measurements to characterize the surface electronic properties of the synthesized films. The results indicated a presence of an amorphous tin oxide layer on the surface. Consequently, we etched the films to remove the surface oxide layer, and identified unexpected high concentrations of oxygen throughout the etched SnS films. As no other crystalline phases could be detected in the bulk of these films, we assume that the oxygen is embedded in the lattice and affects its intrinsic charge carrier concentration. To reduce the oxygen effect on the electronic properties of the SnS films, we improved the solution deposition recipe to achieve a significant reduction of the oxygen content of the film.