2025.

Structure of Te-rich amorphous Ge-Sb-Te alloys

The structure of evaporated amorphous $Ge_xSb_xTe_{100-2x}$ (x = 6, 9, 13) alloys was investigated by neutron diffraction, X-ray diffraction, and extended X-ray absorption spectroscopy at the Ge, Sb, and Te K-edges [1]. Large-scale structural models were generated by fitting the experimental datasets (five for each composition) simultaneously in the framework of the reverse Monte Carlo simulation technique. It was found that the alloys are chemically ordered (Ge and Sb have predominantly Te neighbors) and within the experimental uncertainty, each component satisfies the 8 – N rule. A comparison with the pair correlation functions of melt-quenched $Ge_{20}Te_{80}$ revealed that the first minimum of $g_{TeTe}(r)$ is shallower in the ternary alloys than in $Ge_{20}Te_{80}$. On the other hand, the separation of the first and second coordination environments of Ge atoms is stronger in the Ge–Sb–Te alloys investigated (Figure 1.).

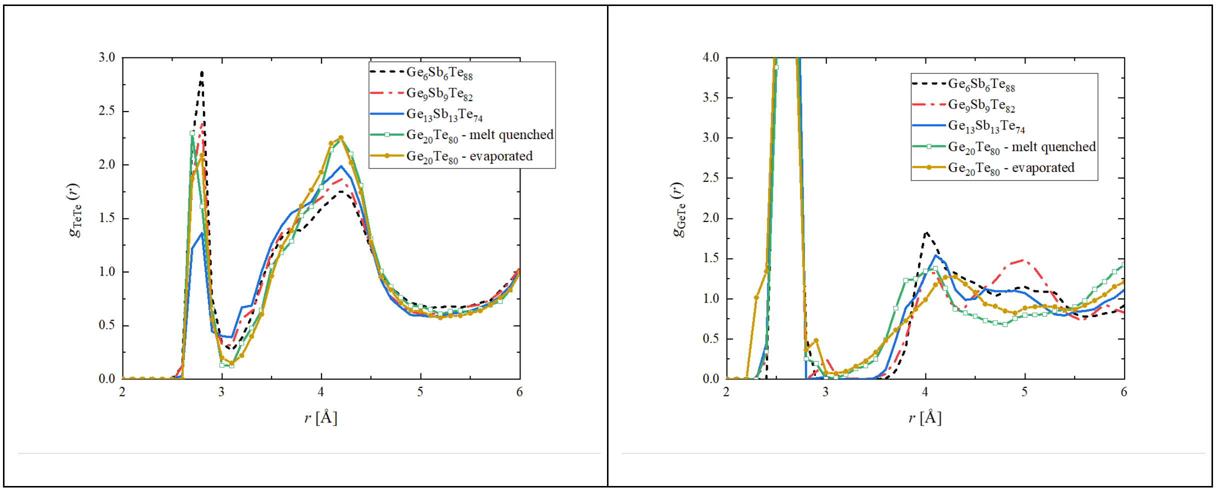

Figure 1. Comparison of the $g_{TeTe}(r)$ (left) and $g_{GeTe}(r)$ (right) partial pair correlation functions of the $Ge_xSb_xTe_{100-2x}$ alloys with those of $Ge_{20}Te_{80}$ and sputtered amorphous $Ge_2Sb_2Te_5$.

Nuclear quantum effects (NQE) in hydrogen bonded liquids

Extensive molecular dynamics (MD) computer simulations have been conducted on ambient neat liquid formamide, $HC(=O)NH_2$, methanol, CH_3-OH, and water, H_2O, using the polarizable AMOEBA force field for each molecule. At room temperature, each of these molecules can form hydrogen bonded networks of varying extent. Nuclear quantum effects have been determined from the classial MD trajectories [2] by applying the 'GSTA' (Generalized Smoothed Trajectory Analysis) scheme [3] introduced recently. In each liquid, intramolecular N-H, O-H and C-H bonds are affected the most by NQE-s, whereas the first intermolecular H-bonding distances are also influenced. Here we demonstrate nuclear quantum effects on higher order correlations, in particular, on the so-called 'Spatial Distribution Functions' (SDF) [4]. SDF-s are calculated from spatial (3D) probabilities of occurrence of molecules in a coordinate system fixed on a molecule in the centre. Using the difference between the original and NQE corrected SDF-s, detailed 3D pictures of the NQE in H-bonded systems can be obtained. In Figure 2., 'difference'-SDF-s are displayed for liquid methanol, formamide and water. It is observed that NQE-s are most significant at larger O...OH angles (blue: negative value in the figures). This picture is consistent with the findings obtained on the basis of other characteristics, e.g., O…OH hydrogen bond angle distributions: the density of neighboring molecules decreases along the direction of the hydrogen bond, whereas it increases in directions somewhat away from the H-bonding axis. In other words, NQE-s smear out the distribution of nearest H-bonded neighbors around a central molecule.

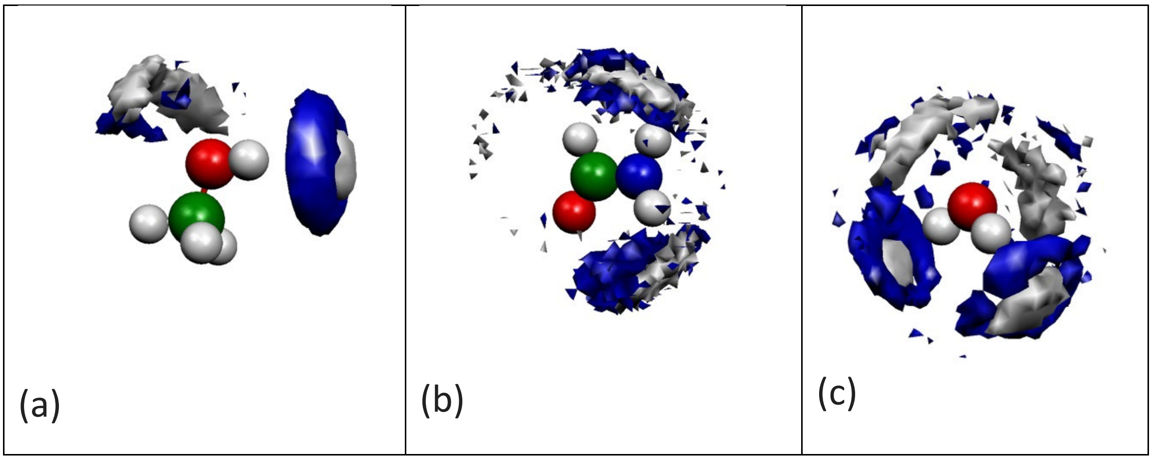

Figure 2. Difference SDF-s (original MD - GSTA corrected) around a central molecule in liquid (a) methanol, (b) formamide and (c) water. (White: positive, blue negative.)

Aqueous Environment Around Cyclodextrins

Molecular dynamics simulations were carried out on aqueous solutions of α-, β-, and γ-cyclodextrins (CD) to investigate the hydration properties of these cyclic oligosaccharides. We used a large number of solvent molecules, which enables us to compare the properties of the water around the CD molecule with those that are further away, and thus are not influenced by it. Water molecules close to the CD molecules, whether located inside or outside the cavity, can interact either hydrophilically through hydrogen bonds (H-bonds) or hydrophobically via van der Waals forces and CH…O interactions. In all three studied CDs, the results indicate that more water molecules are associated through hydrophobic interactions than through hydrogen bonding. The studied hydrogen bond properties show significant differences inside and outside the cavity, and their behavior varies among the three systems [5].

[1] https://doi.org/10.1111/jace.20258

[2] https://doi.org/10.1016/j.molliq.2025.127608

[3] https://doi.org/10.1021/acs.jctc.9b00703

[4] https://doi.org/10.1063/1.465158

[5] https://doi.org/10.1016/j.molliq.2025.128646