Covalent liquids: from Peierls distortion to phase change technology

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Some sp-bonded elements and their alloys display a particularly complex thermodynamic behavior in the liquid state: first order liquid-liquid transition in liquid Phosphorus under pressure, closed loop miscibility gap in liquid STe alloys, reentrant local order upon melting of the GeTe compound, negative thermal expansion (density anomaly) in Te rich GeTe alloys. The academic interest for these systems is now stimulated by the recent development of new data storage technologies (R/W DVDs and PC-RAMs) based on the "phase change" of alloys such as $Ge_2Sb_2Te_5$.
Focusing on two examples, this presentation will show how the atomic structure and thermodynamic properties of these liquids are controlled by their electronic structure. First, combining experimental data (neutron scattering, EXAFS) and first principles molecular dynamics, the density anomaly in liquid GeTe alloys, is shown to be different from what is known for water and other "tetrahedral" liquids: it results from a symmetry recovery of a distorted local octahedral environment. I will then show that distinguishing between tetrahedral and (distorted) octahedral liquids is a useful concept since most of the alloys with good phase change capabilities belong to the second category. This is substantiated by a series of neutron scattering experiments and by first principles molecular dynamics studies of GeSbTe alloys.