

Intrinsic Connection between the Structure and Electronic Anomalies of Vitreous Matter

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We argue that semiconducting quenched liquids and frozen glasses may exhibit a set of peculiar electronic states of topological origin. These states reside at transient strained regions arising during structural reconfigurations between distinct aperiodic states intrinsic to quenched melts. The states are predominantly filled and serve as a non-paramagnetic source of charge carriers that may alone account for the observed magnitude of DC-conductivity. The topological states may be sufficient to account for a number of irradiation-induced phenomena in amorphous semiconductors, including: ESR signal, midgap absorption, distinct types of photoluminescence, and the fatigue of photoluminescence. In addition, the predicted presence of an electronic, nearly temperature-independent contribution to the domain surface tension may account for the apparent disagreement between the kinetic and thermodynamic fragility in chalcogenides. If time allows, I will discuss a novel procedure to map the activated transport in deeply supercooled liquids onto the dynamics of a long range classical Heisenberg model with 6-component spins and anisotropic couplings. This procedure provides a microscopic framework for computing the configurational entropy, the relaxational spectrum, and crystal nucleation rate for specific liquids. Already a mean-field analysis of the spin model demonstrates that the liquid dynamics in fragile and strong liquids occur by the same mechanism, contrary to commonly accepted views.

Theoretical Chemistry Institute Seminar Series