Structure and Electronic Anomalies of Amorphous Matter

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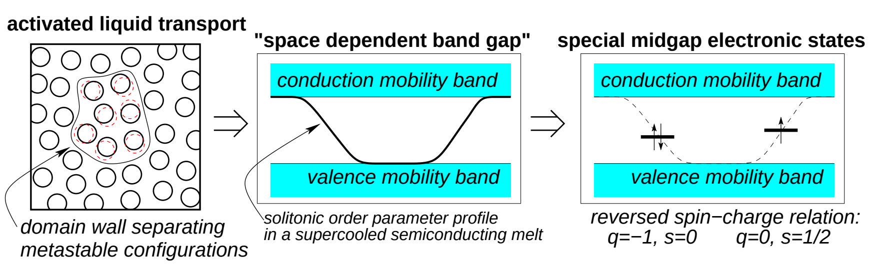
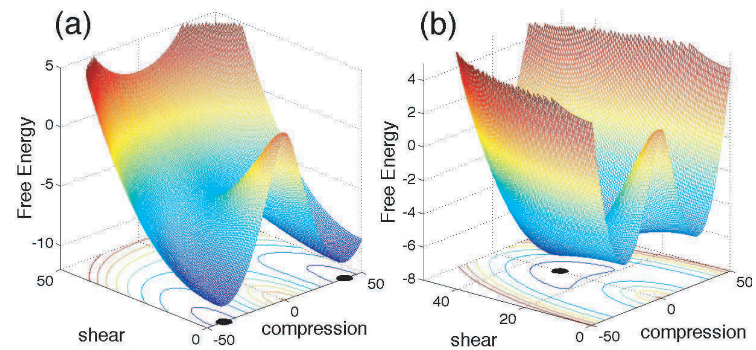
Our long term goal is to develop a self-consistent description of structural and electronic anomalies in several classes of amorphous materials of potential use in energy storage and conversion, including vitreous semiconductors with optical gaps in the visible range and glassy ionic melts. The outstanding questions include the origin and transport of charge carriers in amorphous semiconductors, and the molecular mechanism of conductance in ionic melts. Owing to the exceedingly long relaxation times in these systems and relatively large correlation lengths, there are presently no reliable *ab initio* methods to quantitatively assess the characteristics of the listed materials that are key for their successful application.

1) We have discovered that semiconducting quenched liquids and frozen glasses exhibit a set of peculiar electronic states of topological origin that exhibit a reversed charge-spin relation:



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.

2) We have formulated a novel approach to liquid activated dynamics, in which the activated transitions between the numerous alternative aperiodic configurations are mapped onto the dynamics of a long range classical Heisenberg model with 6-component spins and anisotropic couplings. The spin model exhibits a continuous range of behaviors between two limits corresponding to frozen-in shear and uniform compression/dilation:



The two regimes correspond to strong and fragile liquid behavior respectively; they are separated by a continuous transition controlled by the anisotropy in the spin-spin interaction, which is directly related to the Poisson ratio σ of the material. The latter ratio and the ultra-violet cutoff of the theory determine the liquid configurational entropy. The liquid-to-spin mapping provides a microscopic framework for computing the configurational entropy and relaxational spectrum of specific substances and provides a potential route to obtaining glass structures corresponding to realistic quenching rates.

3) We have computed, on a molecular basis, the viscosity of a deeply supercooled liquid at high shear rates. The viscosity is shown to decrease at growing shear rates, owing to an increase in the structural relaxation rate as caused by the shear. We have explained why the onset of this non-Newtonian behavior occurs universally at a shear rate significantly lower than the typical structural relaxation rate, by about two orders of magnitude.