ELEMENTARY EXCITATION AND ENERGY LANDSCAPE IN SIMPLE LIQUIDS

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The nature of excitations in liquids has been a subject of debate for a long time. In liquids phonons are extremely short-lived and marginalized. Recent research results indicate that instead of phonons local topological or configurational excitations (anankeons) are the elementary excitations in high temperature metallic liquids. Local topological excitations are those which locally alter the atomic connectivity network. They are the atomistic origin of the viscosity in the liquid. They are independent of each other at high temperatures, but interact through the dynamic stress field below the crossover temperature, T_A, resulting in a rapid increase in viscosity, culminating to the glass transition. The crossover phenomenon occurs as a result of the competition between the topological excitations and phonons. The local potential energy of anankeons represents the probability weighted projection of the potential energy landscape (PEL) to the single atom. The PEL is a useful concept, but is highly multi-dimensional and difficult to characterize. A description in terms of the anankeon PEL and their interaction may represent a more effective approach to this complex problem. These discoveries appear to open the way to the explanation of various complex phenomena in liquids, such as atomic transport, fragility, and the glass transition, in terms of these excitations.