**Shear stress correlations and collective excitations in liquid In via ab initio computer simulations**

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A new direction in ab initio studies of condensed matter under pressure is focused on detection of liquid-liquid transitions in metallic liquids as well as on understanding of metal-nonmetal transitions in expanded liquids. Mainly static properties were studied across the liquid-liquid transformation in ab initio simulations, while practically very little information exists in the literature on features in the single-particle and collective dynamics across the transition.

We present an ab initio molecular dynamics study of liquid In within the pressure range from ambient one up to 10 GPa along the melting line. A model system of 300 particles was studied within density functional theory with electron-ion interaction represented by PAW potentials. Radial distribution functions, mean-square displacements, and velocity autocorrelation functions (VACF) are analyzed. The calculated frequency spectrum of VACF reveals two-peak structure, which evolves with pressure. Longitudinal and shear stress-stress autocorrelation functions were calculated from ab initio simulations and the dependence of shear and bulk moduli on pressure was estimated. Longitudinal (L) and transverse (T) collective excitations were observed in the shape of L- and T-current spectral functions. The L and T dispersion curves were estimated and analyzed for increasing pressure. We discuss the correspondence of peaks of frequency spectrum of VACF and flat regions in the obtained T-dispersion curves at different pressures.