What can computer simulation tell about collective excitations in disordered systems that inelastic X-ray scattering experiments cannot ?

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In general, one would actually like to have more information about the collective (vibraional) atomic excitations in disordered materials than for the corresponding crystalline systems: in addition to the spectrum (vibrational density of states, VDOS), one would like to have (as much as possible of) the dispersion relations, $\omega(q)$, knowing which modes are transverse- or longitudinal-like (at low frequencies), all as in the crystalline case. However, disorder causes new phenomena: thus, it is also essential, for example, to know whether modes are spatially localized, and whether a mode frequency is above or below the Ioffe-Regel crossover from weak to strong disorder-induced scattering of plane-wave excitations. Inelastic X-ray (as well as neutron) scattering is good at providing information about the spectrum of (longitudinal) vibrational modes, but provides little information about the nature of the modes themselves.

In this talk, I will briefly review our, and some other, theoretical and computational work on various aspects of collective-mode behaviour in disordered systems. This will include brief discussions on ascertaining the localization-delocalization transition and Ioffe-Regel crossover frequencies, the dispersion relation of v-SiO_2, the origin of the boson peak and disorder-induced zero-energy singularities in the VDOS.