Structure-property relationship is a central issue of materials research. For liquid materials, however, it is difficult to understand how the internal structure influences their properties because it remains an experimental challenge to image the local arrangement of atoms in a disordered system. It is all the more crucial that it is now well accepted that a liquid is not a completely random disordered state but has generally the tendency to have a local structural order. This is particularly true for liquids such as Si and metallic liquids for which ab initio simulations provide direct evidence for the presence of local structural ordering and allow us to study the details of such a structure and its lifetime [1-4]. Such a signature of local structural ordering is found to be more pronounced at lower temperatures, below the melting point $T_m$, in the undercooling regime. However it was also shown that this local structural order can exist even above $T_m$. Transport properties, like the shear viscosity and the diffusion coefficients are kinetic key parameters that determine the crystal nucleation and growth in materials. They also display a very important role in studying the liquid-to-glass transition in a glass-forming system. In experiment the determination of transport properties in the undercooled regime is rather challenging, because any contact of the melt with the container wall immediately induces crystallization of the melt. The convection inside the sample in terrestrial measurements is another problem. Very recently, we have shown that both the shear viscosity and the diffusion coefficients can be determined very accurately for Si and metallic melts using ab initio molecular dynamics [5-8] as well as the hydrogen diffusivity [9]. In this presentation, we will show how the local structural order influences dynamic properties of metallic melts and their evolution as a function of temperature. The relationship between structural and dynamic properties allow us to discuss liquid-solid transition like crystal nucleation and glass formation but also universal laws that relate transport properties to the excess entropy [10].

References