Figure S. 1: Time evolution of the (a) Kinetic Energy and (b) Potential Energy of the system, respectively. The energy is expressed in Atomic Units (a.u.)
We have also analyzed the AIMD trajectory to obtain the time-dependent generalizations of RDFs, namely the van Hove Correlation Functions (VHCF’s) where an additional time dimension, $\tau$ is associated with the RDF’s. The correlation function behaves as normal RDF when $\tau$ acquires a zero value whereas for $\tau > 0$, the observation is performed at fixed position (in our case O atom of NMA) at time 0 and the position of H atom of methanol at time $\tau$ is monitored. Although the NMA is allowed to diffuse, we use the initial position, even though NMA is no longer there. By accepting this criterion, the broadening of the RDF peaks occurs with increasing $\tau$ and at very large value of $\tau$ the functional acquires a value of 1 for all distance $r$. This correlation provides a bridge between experiment and theory as the results from neutron scattering experiments can be plotted as a 3-D plot with frequency on one axis and inverse of distance on another axis. The plot explaining the VHCF’s is shown in Figure S2.

Figure S. 2: van Hove correlation function of O atom of NMA observing H atom of methanol.