Structure and Dynamics of Nanoconfined Liquids
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Dramatic changes in the molecular-level structure and dynamics of liquids occur upon nanoscale confinement in materials ranging from sol-gels to reverse micelles. A number of vibrational and electronic spectroscopic techniques are routinely used to probe the behavior of such nanoconfined liquids. However, in general, what information is contained in the spectra of confined liquids and how the complex molecular-level structural and dynamical properties can be extracted is still an open question. This issue will be discussed in the context of molecular dynamics simulations by examining the affected liquid properties and, when possible, the predicted spectroscopic signals for mesoporous amorphous silica systems. These confining frameworks have been relatively well characterized experimentally, present different surface chemistries, and are sufficiently transparent to permit the study of their contents by a variety of spectroscopies. A particular focus will be the molecular-level origins of the modified liquid behaviour, including those relevant to chemical processes, e.g., reorientational and hydrogen-bond dynamics.