A molecular dynamics study of water molecules with silica surface in chromatographic system

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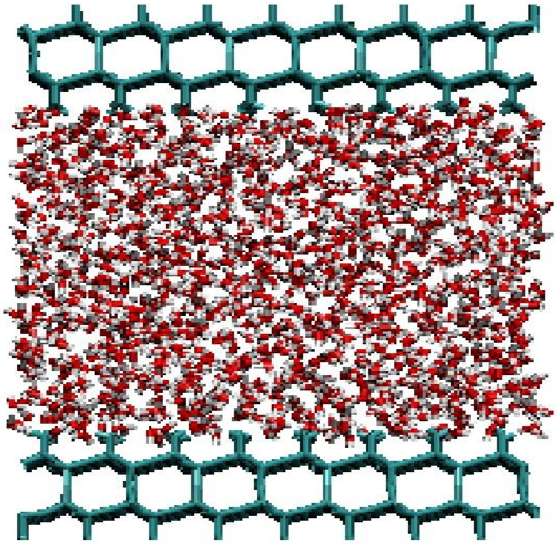
Besides its function as a solvent, water is known to play an active functional role in biological and chemical systems. However, complex systems including chromatographic systems are highly influenced by the amount of water present between the silica layers. The dynamics and ordering is different due to different interfacial regions and intermolecular interactions at the surface[1], e.g. -OH groups of silica surface and the hydration sites in lipid bilayers[2]. Due to this reorganisation dynamics it becomes difficult to study such a system by standard structural techniques such as X-ray or NMR spectroscopy.



Owing to the great practical relevance of Reversed phase liquid chromatography (RPLC), a more detailed study of water dynamics, energetics and the morphology in the stationary phase and at interfaces is carried out by molecular dynamics (MD) simulations. In this work we investigate exchange dynamics of water between the surface-region and the bulk[3] and the H-bond structures, dynamics at water/silica interface[4], because it selectively captures the interfacial dynamics and contribute to their stability and functionality through hydrogen bond interaction[5]. Such a study reveals the temporal evolution of this complex system at an atomistic level.

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