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Confined fluids studied by total neutron scattering

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A lot of processes in applied sciences based on surface chemistry phenomena utilise porous solid materials to increase the accessible surface area. For instance, a mesoporous silica MCM-41 is used as new drug delivery systems for ibuprofen, a more sustainable solution for separation of ethane from natural gas and a heterogeneous catalyst in hydrogenation of benzene. In all of these systems fluid-interface play a key role, however it should be acknowledged that the pores are normally filled up by fluid molecules (i.e. confined fluid).
Nano-confined fluids often have different macroscopic properties than unrestricted bulk corresponding forms. For example, the mobility of molecules is supressed across the whole range of temperatures when liquid benzene is confined in MCM-41.[1] Some studies also suggest an interesting phenomena occurring upon confining miscible in bulk mixtures –a microphase separation of e.g. tert-butyl alcohol and toluene.[2] These discrepancies originate at the molecular level, and total neutron scattering is an exceptional experimental technique giving an access to this information.
Wide Q-range total neutron scattering (0.01 to 50 Å−1) accessible at the NIMROD instrument based at ISIS Neutron and Muon Source has been employed to obtain insights into the structural properties of aliphatic and aromatic hydrocarbons such as benzene-d6, cyclohexane-d12, cyclohexene-d10 confined in the pores of MCM-41.[3] Other studies include understanding the structural properties of a range of gases in MCM-41 (oxygen, nitrogen, deuterium, and deuteriated methane),[4] structure of water in MCM-41[5] and arrangement of benzene and cyclohexane molecules during a reaction on Pt-doped MCM-41.[6]
In this study, scattering data were collected for a set of systems: (i) empty MCM-41, and (ii) MCM-41 loaded with a hydrocarbon. To analyse the data, two atomistic models were constructed –first to represent the confining matrix alone, and a subsequent containing also benzene molecules. Through the refining procedure, the molecules within the simulation box were moved towards the new positions allowing for mimicking the collected scattering patterns. The final model of the system is used to calculate structural properties of the confined liquid such as radial and angular distribution functions, spatial density functions, distribution of molecules across a pore.
The results obtained for benzene confined in MCM-41 showed that the some weak interactions that are responsible for 'ordering'of molecules within the bulk liquid benzene seem to be drastically altered by the presence of the constraining interface. The further studies on how the chemical nature of the surface of the confining matrices and their pore size affect the structural properties of confined fluids are ongoing. Understanding the confinement effects on fluids structure is crucial for a conscious tailored design of systems and processes involving them, such as membranes for removal of pollutants from water, systems controlling the fate of drugs within the patients, oil in porous shales, permeable anodes and cathodes in fuel cells and CO2 captured and stored within nano-cages in Metal Organic Frameworks, to name but a few.

Participation

In-Person

References

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