

Fluids confined in random porous media: Some recent progresses

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In this talk, we present some recent progresses in the study of fluid adsorption in random porous matrices in two directions. The first concerns the development of some analytical equations of state. Although intense investigations have been made during the last two decades, no analytical result has been found for any non trivial off-lattice model for fluids in random porous media. Recently, we have succeeded in extending the scaled particle theory to a HS fluid confined in some model matrices. The agreement between our SPT and simulation results is fine (errors $\leq 20\%$). An empirical correction to the SPT was found which leads to a highly accurate EOS over the whole density range with errors comparable to the simulation ones.

In the second part of the talk, we will present some results on the study of hard sponge model. The morphology of many porous materials is sponge-like. Despite the abundance of such materials, simple models which allow for theoretical description of these materials have been proposed only recently [1]. Ornstein-Zernike type integral equations have been formulated for this model. The numerical solution of these equations requires closure relations between total and direct correlation functions. Although HNC and PY like closures can be formulated also for the hard sponge model, we will show that these popular closures for bulk fluids have serious flaws for the fluids confined in a hard sponge matrix. Some possible strategies for formulating appropriate closures will be discussed.

1. S.L. Zhao, W. Dong and Q.H. Liu, Fluids in porous media: 1. A hard sponge model. *J. Chem. Phys.* **125**, 244703, (2006).