数学与系统科学研究院

计算数学所学术报告

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报告题目：

Theoretical Study of Hard-Sphere Fluid Mixtures Confined in Porous Media

邀请人：　卢本卓 研究员

报告时间：**2016** 年 **6** 月 **13** 日（周一）

上午 **10:00-11:00**

报告地点：　数学院南楼七层

702 会议室

Abstract:

Porous materials have important technological applications such as molecular sieve, catalyst, chemical sensor, etc. In recent years, there have been considerable investigations for understanding thoroughly the structure of these materials as well as the behavior of substances confined in them. Much effort (both experimental and theoretical) has been devoted to the study of porous materials. In their pioneering work, a very simple model for the fluid adsorption in random porous media was proposed by Madden and Glandt. The matrix in Madden-Glandt model is made by quenching an equilibrium system. Then, a fluid is adsorbed in such a matrix.

Recently, T. Patsahan, M. Holovko and W. Dong have extended the scaled particle theory (SPT) to confined fluids and derived analytical equations of state (EOS) for a hard sphere (HS) fluid in some matrix models. By using SPT method, I obtained the equation of state of additive hard-sphere (AHS) fluid mixtures confined in porous media. The contact values of the fluid-fluid and fluid-matrix radial distribution functions (RDF) were derived as well. The results of the contact values of the RDFs and the chemical potentials of different species were assessed against Monte Carlo simulations.

Moreover, I analyzed also the fluid-fluid phase separation of non-additive hard sphere (NAHS) fluid confined in porous media. An equation of state is derived by using a perturbation theory with a multi-component fluid reference. The results of this theory are in good agreement with those obtained from semi grand canonical ensemble Monte Carlo simulations.

欢迎大家参加！