RESEARCH PAPERS

硬球链流体在狭缝中密度分布的Monte Carlo模拟

王丙强, 蔡钧, 刘洪来, 胡英

Department of Chemistry, East China University of Science and Technology, Shanghai 200237, China

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摘要　Covering a wide range of bulk densities, density profiles for hard-sphere chain fluids (HSCFs) with chain length of 3,4,8,20,32 and 64 confined between two surfaces were obtained by Monte Carlo simulations using extended continuum configurational-bias (ECCB) method. It is shown that the enrichment of beads near surfaces is happened at high densities due to the bulk packing effect, on the contrary, the depletion is revealed at low densities owing to the configurational entropic contribution. Comparisons with those calculated by density functional theory presented by Cai et al. indicate that the agreement between simulations and predictions is good. Compressibility factors of bulk HSCFs calculated using volume fractions at surfaces were also used to test the reliability of various equations of state of HSCFs by different authors.

关键词　molecular simulation　Monte Carlo method　hard-sphere chain fluid　density profile　density functional theory　compressibility factor

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Monte Carlo Simulations of Density Profiles for Hard-Sphere Chain Fluids Confined Between Surfaces

WANG Bingqiang, CAI Jun, LIU Honglai, HU Ying

Department of Chemistry, East China University of Science and Technology, Shanghai 200237, China

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Abstract Covering a wide range of bulk densities, density profiles for hard-sphere chain fluids (HSCFs) with chain length of 3,4,8,20,32 and 64 confined between two surfaces were obtained by Monte Carlo simulations using extended continuum configurational-bias (ECCB) method. It is shown that the enrichment of beads near surfaces is happened at high densities due to the bulk packing effect, on the contrary, the depletion is revealed at low densities owing to the configurational entropic contribution. Comparisons with those calculated by density functional theory presented by Cai et al. indicate that the agreement between simulations and predictions is good. Compressibility factors of bulk HSCFs calculated using volume fractions at surfaces were also used to test the reliability of various equations of state of HSCFs by different authors.

Key words molecular simulation; Monte Carlo method; hard-sphere chain fluid; density profile; density functional theory; compressibility factor

通讯作者:
王丙强
作者个人主页: 王丙强; 蔡钧; 刘洪来; 胡英

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