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Comparison of perturbation theory and mean spherical approximation based on molecular simulation data

刘文彬, 李以圭, 陆九芳

Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

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摘要 A comprehensive study on various internal energies for the dipolar hard sphere fluids, including Stockmayer fluids, the mixtures of Lennard-Jones and Stockmayer and Stockmayer fluids and the electrolyte solutions is reported based on the perturbation theory and mean spherical approximation. Compared with the results of molecular simulations, it is shown that the perturbation theory is better than the mean spherical approximation.

关键词 <u>perturbation theory</u> <u>mean spherical approximation</u> <u>molecular simulation</u> <u>internal energies</u>

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Liu Wenbin, Li Yigui, Lu Jiufang

Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

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Key words perturbation theory; mean spherical approximation; molecular simulation; internal energies

通讯作者:

刘文彬

作者个人主页: 刘文彬; 李以圭; 陆九芳

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