

## THERMODYNAMICS

密度泛函理论在非极性纯流体表面性质研究中的应用

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**摘要** The density functional theory, simplified by the local density approximation and mean-field

approximation, is applied to study the surface properties of pure non-polar fluids. A reasonable long rang correction is adopted to avoid the truncation of the potential. The perturbation theory is applied to establish the equation for the phase equilibrium, in which the hard-core chain fluid is as the reference fluid and the Yukawa potential is used as the perturbation term. Three parameters,  $\epsilon$ ,  $d$  and  $m_s$ , are regressed from the vapor-liquid equilibria, and the surface properties, including density profile, surface tension and local surface tension profile are predicted with these parameters.

**关键词** [表面性质](#) [密度函数理论](#) [无极性流体](#) [表面张力](#) [分子模拟技术](#)

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### Study on Surface Properties for Non-polar Fluids with Density Functional Theory

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**Abstract** The density functional theory, simplified by the local density approximation and mean-field approximation, is applied to study the surface properties of pure non-polar fluids. A reasonable long rang correction is adopted to avoid the truncation of the potential. The perturbation theory is applied to establish the equation for the phase equilibrium, in which the hard-core chain fluid is as the reference fluid and the Yukawa potential is used as the perturbation term. Three parameters,  $\epsilon$ ,  $d$  and  $m_s$ , are regressed from the vapor-liquid equilibria, and the surface properties, including density profile, surface tension and local surface tension profile are predicted with these parameters.

**Key words** [density functional theory](#); [surface tension](#); [density profile](#); [pure non-polar fluids](#)

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