Phase behavior of simple fluids and binary symmetric mixtures in pillared slit-like pores: A density functional approach

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Density functional approach is applied to study the phase behavior of Lennard-Jones(12,6) fluids and their binary mixtures in pillared slit-like pores. Our focus is in the evaluation of phase transitions in fluid adsorbed in the pore of a fixed width. If the length of pillars is sufficiently large, we observe additional phase transitions of the first and second order due to the symmetry breaking of the distribution of chain segments and fluid species with respect to the slit-like pore center. Re-entrant symmetry changes and additional critical, critical end points and tricritical points then are observed. The scenario of phase changes is sensitive to the energy of fluid-fluid and fluid-solid interaction, the amount, and the length of the pillars. Quantitative trends and qualitative changes of the phase diagrams topology are examined depending on the values of these parameters