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Phase behavior and mixing-demixing transitions in binary liquid mixtures with spherical and non-spherical interactions[1] ENRIQUE DIAZ-HERRERA, Depto. de Fisica, UAM-I (MEXICO), GUILLERMO RAMIREZ-SANTIAGO, Instituto de Fisica, UNAM (MEXICO), J. ANTONIO MORENO-RAZO, Depto. de Fisica, UAM-I (MEXICO) — We have carried out extensive equilibrium molecular dynamics simulations to study the temperature versus density phase diagrams and the mixing-demixing transition line in fluid equimolar binary mixtures modeled by: (i) Lennard-Jones, (ii) Stock-Mayer, and (iii) Gay- Berne molecular interactions. These studies are performed as function of miscibility parameter, $\alpha = \epsilon_{AB}/\epsilon_{AA}$, where $\epsilon_{AA} = \epsilon_{BB}$ and ϵ_{AB} stand for the parameters related to the attractive part of the intermolecular interactions for similar and dissimilar particles, respectively. When the miscibility of the Lennard-Jones mixture varies in the range $0 < \alpha < 1$, a continuous critical line of consolute points $T_{\rm cons}(\rho)$, appears. This line intersects the liquid-vapor coexistence curve at different positions depending on the values of α, yielding mainly three different topologies for the phase diagrams. These results are in qualitative agreement to those found previously for square well and hard-core Yukawa binary mixtures. We also carry out a detailed study of the liquid-liquid interfacial and liquid-vapor surface tensions, as function of temperature and miscibility as well as its relationship to the topologies of the phase diagrams. Similar studies and analysis are also performed for Stock-Mayer and Gay-Berne binary mixtures.

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Enrique Diaz-Herrera
Depto. de Fisica, UAM-I (MEXICO)

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