

Associating fluid theory for an explicit hard spherocylinder solvent ionic model in a disordered porous matrix

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We have developed a theoretical approach to describe the thermodynamic properties of the ionic solution modelled by the primitive model with an explicit consideration of the neutral hard spherocylinder solvent. The solution is studied in a disordered porous confinement presented as a uniform dispersion of immobile spherical particles (Figure 1). The proposed theory is based on a combination of two approaches: the scale particle theory for the description of the reference system represented by a mixture of hard spheres and prolate hard spherocylinders immersed in a matrix [1] and the associative mean-spherical approximation for taking into account Coulomb interactions between ions [2]. For the considered solvent explicit model in a matrix, analytical expressions for pressure, free energy and partial chemical potentials are derived for the first time [3]. Using these expressions, the liquid-liquid phase transition is studied, where one phase is enriched with ions and another one – with solvent particles. In the solvent-rich phase, the isotropic-nematic phase transition is observed due to the orientational ordering of the spherocylinder solvent particles at different porosities of a matrix. The effects of the matrix confinement and of the solvent particle elongation on the liquid-liquid and isotropic-nematic phase transitions are studied at different pressures. The role of association phenomena appearing between positively and negatively charged ions in phase behavior of the considered ionic solutions under confinement is discussed.

REFERENCES

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FIGURES

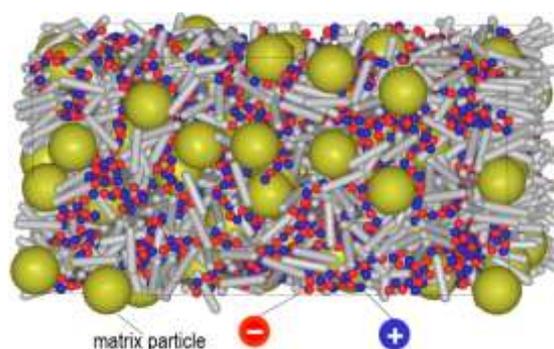


Figure 1: Hard spherocylinder solvent ionic model in a disordered porous medium