

USING MOLECULAR DYNAMICS TO STUDY PHASE EQUILIBRIUM WITH DIRECT COEXISTENCE METHODS

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The coexistence of various different phases is such a quotidian phenomenon as to produce the folk wisdom phrase “water and oil don't mix”. The hidden complexity of that simple statement can be appreciated in the very existence of living organisms: cell membranes separate an “inner” aqueous solution from an “outer” one, each having a different concentration of the same solutes. Whereas the advancement of molecular models employed in numerical simulations now allows for the study of phospholipid bilayers, for instance, there is still no agreement on the ability of force-fields to correctly reproduce the melting temperature of ice, or the solubility of salts. The use of direct coexistence methods in the theoretical study of these latter two phenomena will be discussed in this talk, as well as the effects produced by the influence of an external electric field.