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Molecular Dynamic Simulations in Binary Liquid Mixtures

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Experimental data of liquid binary mixtures can provide the thermodynamic and transport properties[1]. Molecular dynamics simulations (MD) are preformed on the same mixtures at the same experimental conditions: at different temperatures and different mixture compositions. Molecular dynamics simulations can gain a deeper understanding of the behavior of liquid mixtures at the molecular level. It can be used for analyzing specific properties, such as the radial distribution functions (RDFs), interactions in the mixture, thermodynamic and transport properties, understanding the dynamics of the system.This information can be used to obtain insight into the molecular level, to understand the nature of the interaction and to predict the behavior under specific conditions. The right force field are essential for describing the system and using the density of the simulated systems as a represented data to compare to the experimental data. We performed experimental measurements and molecular dynamics simulations on four systems to study influence of double bonds on the properties of alcohol mixtures. The data of the molecular dynamic simulations are in an agreement with the data from experimental measurement, and at the same time we can observe interactions at the molecular level that indicate different noncovalent interactions of double bonds in comparison with single bonds.

Keywords: binary mixtures, thermodynamic properties, molecular dynamic simulations

References

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