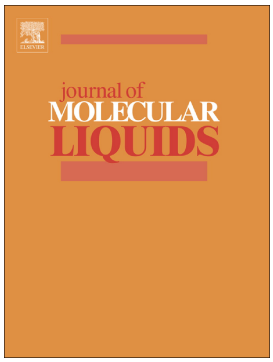

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Importance of Nanolayer Formation in Nanofluid Properties: Equilibrium Molecular Dynamic Simulations for Ag-Water Nanofluid

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Abstract

Most of the researches have authenticated the irrefutable role of interfacial nanolayer in molecular level. Understanding the mechanism of interfacial nanolayer effect on macroscopic fluid properties is of crucial importance. Thus, this study is aimed to examine the effect of nanolayer on two important nanofluid properties, i.e. density and viscosity, by performing extensive molecular dynamics simulations. It was found that, the formation of the ordered liquid nanolayer caused contraction of base fluid. The nanofluid was considered as a three-component mixture, i.e. nanoparticle, base fluid after mixing with nanoparticles and nanolayer. Accordingly, a new ternary mixture relation was proposed to compute the nanofluid density. Obtained results revealed the importance of nanolayer effect on density of nanofluids. Moreover, the role of liquid layering in nanofluid viscosity was analyzed. The obtained results can provide useful understanding on the structural and transport properties of nanofluids not only in the Ag-water nano-colloid, but also in other types of nanofluids.

Keywords: Silver nanofluid; liquid layering; Equilibrium molecular dynamics; Density; Viscosity; ternary mixture

1. Introduction

Recognition of nanoscale mechanisms is crucial to provide a better explanation for nanocolloids properties. The interfacial nanolayer is one of the most important nanoscale mechanisms playing a significant role in thermophysical properties of nanofluids. Coulomb or van der Waals interactions at solid-liquid interface tend to form a dense liquid layer which