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The Molecular dynamics study of atomic Management and thermal behavior of Al-Water Nanofluid: A two phase unsteady simulation

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Abstract

Molecular Dynamic (MD) approach is used to describe the temperature and pressure effects on the Al nanoparticles aggregation process in the aqueous environment of water as the base liquid. For this goal, various physical parameters like total energy, temperature, aggregation time, and total energy of the simulated structures, are reported. The results show that the aggregation process enlarges by the ratio of temperature and pressure. By atomic mobility increasing, the Al nanoparticles collide with each other in a shorter simulation time. Numerically, by temperature increases from 300K to 350K, the aggregation time decreases from 1.33ns to 1.18ns. Furthermore, aggregation time increases to 1.99ns by more pressure to 5bar.