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Molecular Dynamic Simulations on Surface Tension of Methanol[1]

ABDALLA OBEIDAT, Jordan University of Science and Technology — Molecular dynamic simulations have been performed to study the surface tension of methanol at low temperatures. Six different models of methanol have been studied to compute the surface tension of different models. The models have been used to predict the surface tensions are: OPLS, Gromos 96, H1, J1, J2, and van Leeuwen model. Our results show that the most accurate model compared to true methanol was van Leeuwen model. The results were fitted to a straight line to predict other data of surface tension at specific temperature. The simulation were performed using the Gromacs package at temperatures: 200, 210, 220, 230, 240, 250, 260, 270, 280, 290, and 300 K.

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