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Surface Tension of Alcohol-Water Mixtures Using Molecular Dynamics Simulations. ABDALLA OBEIDAT, HIND ABU-GHAZLEH, Jordan University of Science and Technology — Molecular dynamics is used to calculate the surface tension of alcohol-water mixtures. The gromos force fields of united atoms and all atoms of alcohols (methanol, ethanol, propanol, and acetone) has been used. The surface tension of alcohols has been calculated at different temperatures ranges from 200-300K, while for mixtures, the surface tension has been calculated at 298K with different concentrations. In all simulations, Gromacs is used with periodic boundary conditions in all dimensions. The simulated results are compared with the experimental values in literature, and with Monte-Carlo simulations as well.

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