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Surface Tension of Methanol as a Function of cut-off Radius and Temperature Controllers.[1] ABDALLA OBEIDAT, ADNAN JARADAT, BUSHRA HAMDAN, JUST — Molecular dynamics is used to calculate the surface tension of van Leeuwen methanol. The van Leeuwen model of methanol is chosen over other models of methanol, since this model is widely used to study nucleation at low temperature. Usually, scientists use the cut-off radius to be three order of magnitude of segment diameter. In this study, we varied the cut-off radius to estimate the best cut-off at which the surface tension reaches its plateau. After deciding the best cut-off radius for van der Waals and Coulomb interactions (CUT-OFF and PME were used for Coulomb interaction), we varied the temperature controller (van-Housen, Berendsen, and v-rescale) to decide the best temperature controller to be used to study methanol. In all simulations, Gromacs is used at T=200-300K with periodic boundary conditions in all dimensions.

[1]JUST

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