

5. Liquid crystal phase and water-like anomalies in a core-softened shoulder-dumbbells system

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Using molecular dynamics we investigate the thermodynamics, dynamics and structure of 250 diatomic molecules interacting by a core-softened potential. This system exhibits thermodynamic, dynamic and structural anomalies: a maximum in density-temperature plane at constant pressure and maximum and minimum points in the diffusivity and translational order parameter against density at constant temperature. Starting with very dense systems and decreasing density the mobility at low temperatures first increases, reaches a maximum, then decreases, reaches a minimum and finally increases. In the pressure-temperature phase diagram the line of maximum translational order parameter is located outside the line of diffusivity extrema that is enclosing the temperature of maximum density line. We compare our results with the monomeric system showing that the anisotropy due to the dumbbell leads to a much larger solid phase and to the appearance of a liquid crystal phase.