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Computer simulation study of the molecular dynamics in homocysteine systems

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Excessive amount of homocysteine in the human body have been recently considered as a factor which increases the risk of the developing of cardiovascular diseases. The pure clusters composed of a finite number n = 30, 65, 140, 860 and 2500 of homocysteine molecules have been studied by MD technique. Moreover, the same clusters surrounded by water have been also investigated. The mean square displacement, diffusion coefficient, radial distribution function and the Lindemann index of homocysteine molecule have been calculated for several temperatures, including the physiological temperature T = 310 K.
The physical observables and snapshots of instantaneous configurations for pure homocysteine clusters and the systems with water are presented and interpreted.
The dynamics of homocysteine in pure clusters and in the systems with water varies substantially.