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Ethane clathrates using different water-ethane models: Molecular dynamics

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HIGHLIGHTS

The performance of different water models in ethane clathrates was analysed by molecular dynamics simulations. The study was carried out inside of the temperature regime where a stable-unstable transition takes place.

None of the considered water models was able to reproduce the transition temperature by using the standard Lorentz-Berthelot combining rules.

The current manuscript shows that a slight modification on combining rules allows us to approach to the experimental temperature. By modifying both cross terms, the intensity of attraction and the average size of atoms, the decomposition of ethane clathrates was observed.

Such process was evidenced by monitoring the coordination number, hydrogen bonds, radial distribution functions, mean force potential and the mean square displacement. Based on these results we mentioned that the entropic effects are also important as enthalpic ones.

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