GENERALIZED STILLINGER–DAVID POTENTIAL

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S u m m a r y

We present an improved version of the Stillinger–David polarization potential of the intermolecular interaction in water. A clear algorithm of construction of a function describing the oxygen-hydrogen interaction in water molecules is formulated. A new approach to the modeling of a function screening the charge-dipole interaction on small distances is developed. To describe the long-range asymptotics of the intermolecular potential, the bare Stillinger–David potential is supplemented by a term related to the interaction of dipole moments of oxygen ions. In addition, we introduce a term involving a deformation of the electron shells of oxygen ions to the polarization component. These corrections allow us to successfully reproduce all essential results of quantum mechanical calculations of the interaction energy for water molecules obtained by Clementi. Analyzing the behavior of the dipole moment of a water molecule as a function of the intermolecular distance, we obtain the estimate of irreducible two-particle effects in water.