

Molecular Dynamics Study of Gases H_2 , D_2 and T_2

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Abstract: The classical molecular dynamics simulation has been used to study the equation of state of gas H_2 , D_2 and T_2 . It has also been investigated that the isotope mass affects on the accuracy of equation of state. Our calculated results show that the classical effect is principal and the isotope mass effects on the equation of state are obvious for the much light gases. At the same time, some useful theoretical data of equation of state for these gases have been provided. It is found that the classical simulation is still effective to the quantum gas. However, the quantum mechanics simulation and the improvement of intermolecular interaction potential are necessary if more accurate computational results are expected.

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Key words: molecular dynamics simulation, equation of state, hydrogen and its isotope gases, interaction potential, isotope mass effect

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