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Abstract

The theory of statistical thermodynamics reproduces the macroscopic properties of matter based on the microscopic molecular interactions. This depends on the statistical laws which produce the complex behavior of the macroscopic systems from the simpler interaction potentials. The theory predicts the state laws, the mean molecular structure and the dynamics of matter. Conversely, the macroscopic data can be reduced to microscopic information such as the intermolecular potentials. The latter can be used for the calculation of other equilibrium and kinetic properties of matter. The theory is applied to

molecular systems in equilibrium, such as the ideal and real gases, liquids, crystals, electron and phonon gases, quantum systems, etc

Similarly, the development of computer programming permits the simulation of thermodynamic systems with the calculation of the particle positions in time and their analysis based on statistical mechanics. This new approach for the calculation of macroscopic properties through molecular dynamics simulation and the stochastic Monte Carlo method is useful for the prediction of properties and the determination of microscopic interactions from experimental data.



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