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Molecular gas dynamics : theory, techniques, and ...

Date: Topics . Reference: 8/22: Molecular hypothesis. Elementary gas kinetic theory. Pressure. Avogadro's law. Temperature. Gas constants and molecular quantities.

AAE590D: Molecular Gas Dynamics

1) Calculate basic gas properties such as temperature, pressure, flow velocity, gas stresses and fluxes from the molecular velocity distribution function. 2) Identify gas flow regimes (continuum, slip, transitional, free molecular) and applicable governing equations. 3) Apply equilibrium fluxes to solve basic free-molecular flow problems.

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Based on the molecular dynamics theory, the transport process of methane in carbon nanopores was studied, including simulation of the arrangement of the wall atoms, slip and transitional flow of methane in the supercritical state and application of different driving forces.

Molecular dynamics simulation of methane gas flow in ...

The quantum calculations covered involve Hartree-Fock molecular orbital (HF-MO), Generalized Valence Bond (GVB) [49, 50] and the Complete Active Space Self-consistent Filed (CASSCF) [50, 51], and full CI methods. [51] Density Functional Theory (DFT) calculations [52-54] are also incorporated into AIMD.

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AAE590D: Molecular Gas Dynamics

At the molecular level, gas dynamics is a study of the kinetic theory of gases, often leading to the study of gas diffusion, statistical mechanics, chemical thermodynamics and non-equilibrium thermodynamics. Gas dynamics is synonymous with aerodynamics when the gas field is air and the subject of study is flight.