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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 Field (CASSCF) [50, 51], and full CI methods. [51] Density Functional Theory (DFT) calculations [52-54] are also incorporated into AIMD.

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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-

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equilibrium thermodynamics. Gas dynamics is synonymous with aerodynamics when the gas field is air and the subject of study is flight.

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