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Tautomeric equilibrium in condensed phases | Journal of Chemical Theory and Computation We present an ab initio molecular dynamics (MD) investigation of the tautomeric equilibrium for aqueous solutions of glycine and acetone at realistic experimental conditions. Metadynamics is used to accelerate proton migration among tautomeric centers.

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Condensed FUS LC values are between -1 and 1, indicating that disorder is preserved in the condensed phase, while chemical shifts in the fibrillar form are closer to values associated with β ...

Molecular interactions underlying liquid–liquid phase ...

Molecular Kinetics in Condensed Phases: Theory, Simulation and Analysis puts the focus on the theory, algorithms, simulations methods and analysis of molecular kinetics in condensed phases. The authors - noted experts on the topic - offer a detailed and thorough description of modern theories and simulation methods to model molecular events.

Molecular Kinetics In Condensed Phases - By Ron Elber ...

The uniform approach and common language used in all discussions help to develop general understanding and insight on condensed phases chemical dynamics. The applications discussed are among the most fundamental processes that underlie physical, chemical, and biological phenomena in complex systems.

Chemical Dynamics in Condensed Phases: Relaxation ...

This thesis presents the ring polymer molecular dynamics (RPM) approximation to the Kubo-transformed time correlation function and shows how it may be used as the basis of an approximate quantum-mechanical method for determining the dynamical properties of condensed-phase molecular systems.

Ring polymer molecular dynamics

Chemical dynamics in condensed phases : relaxation, transfer and reactions in condensed molecular systems. Responsibility. Abraham Nitzan. Imprint. Oxford ; New York : Oxford University Press, 2006. Physical description. xxii, 719 p. : ill. 25 cm. Series. Oxford graduate texts.

Chemical dynamics in condensed phases : relaxation ...

In particular, our studies deal with chemical processes involving interactions between light and matter, chemical reactions in condensed phases and at interfaces and transport phenomena in complex systems, focusing mainly on the following directions: Energy transfer processes in molecular systems. Molecular dynamics in condensed phases.

Abraham Nitzan | Department of Chemistry

FEMTOSECOND CHEMICAL DYNAMICS IN CONDENSED PHASES 145 relaxation is typical for many liquids. Aside from the good correspon- dence of the simulation and experiment, it is noteworthy how rapid the initial phase of the relaxation is. More than 50% of the relaxation is complete in less than 55 fs.

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