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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.

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This thesis presents the ring polymer molecular dynamics (RPMD) 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.