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Chapter 1 : Advanced Modeling Reactive Molecular Dynamics Modeling

A comprehensive, in-depth presentation of theoretical underpinnings and mathematical techniques This is the first book of its kind to combine all the theories of molecular reaction dynamics and chemical kinetics in a single source.

Show Context Citation Context However, one cannot always assume separation of timescales. It has been shown that a conformational transition or rea Truong , " It is based on canonical variational transition-state. Conventional transition-state theory TST with one-dimensional Wigner or Eckart tunneling corrections is also available. Potential energy information needed for the rate calculations are obtained from ab initio molecular orbital andror density functional electronic structure theory. Vibrational-state-selected rate constants may be calculated using a diabetic model. TheRate also introduces several technical advancements, namely the focusing technique and energy interpolation procedure. The focusing technique minimizes the number of Hessian calculations required by distributing more Hessian grid points in regions that are critical to the CVT and tunneling calculations and fewer Hessian grid points elsewhere. The energy interpolation procedure allows the use of a computationally less demanding electronic structure theory such as DFT to calculate the Hessians and geometries, while the energetics can be improved by performing a small number of single-point energy calculations along the MEP at a more accurate level of theory. The CH q H l CH q H reaction is used as a model to demonstrate usage of the4 3 2 program, and the convergence of the rate constants with respect to the number Time-dependent studies of reaction dynamics: Mccoy , " In our formulation, the initial conditions for the classical degree of freedom are chosen from the phase space probability distribution given by the Wigner transform of the wave function that was used in the quantum simulation. The conformational equilibria of MgATP in solution is studied using molecular dynamics MD augmented with umbrella sampling methods. Free energy comparisons show that the Mg ion is equally likely to coordinate the oxygens of the two end phosphates, or of all three phosphates. The MD trajectories reveal two major degrees of freedom of the MgATP molecule in solution, and we compute the free energy as a function of these variables, and determine its elastic properties. Comparing the free energy function with several crystallographic structures of ATP analogs, we find that the crystal structures correspond to states where ATP would be elastically strained. The average water density around MgATP is investigated to show the average number of hydrogen bonds and the hydrophobicity. Jansen , " We investigate how accurate different methods of the spectral line shape analysis work in two-dimensional correlation spectroscopy 2D CS for systems with non-Gaussian dynamics. A direct link is established between the frequency dependent correlation functions and a number of line shape m A direct link is established between the frequency dependent correlation functions and a number of line shape metrics. Two model systems are constructed mimicking a typical molecular system with conventional Gaussian and non-Gaussian spectral dynamics. The frequency dependent correlation function and several line shape parameters extracted from the 2D CS spectra at different waiting times reveal dissimilar dynamics in different frequency domains in the non-Gaussian case and similar dynamics in all domains in the Gaussian case. The extracted frequency dependent correlation times agree well with the local dynamics in the underlying model for all analysis methods. We also find an extension of the existing line shape analysis methods that allows the extraction of the third-order correlation function. Within the experimental uncertainties theoretical and experimental results are compatible with each other.

Chapter 2 : Comparison of software for molecular mechanics modeling - Wikipedia

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In many-body potentials, the potential energy cannot be found by a sum over pairs of atoms, as these interactions are calculated explicitly as a combination of higher-order terms. In the statistical view, the dependency between the variables cannot in general be expressed using only pairwise products of the degrees of freedom. For example, the Tersoff potential , [31] which was originally used to simulate carbon , silicon , and germanium , and has since been used for a wide range of other materials, involves a sum over groups of three atoms, with the angles between the atoms being an important factor in the potential. Other examples are the embedded-atom method EAM , [32] the EDIP, [30] and the Tight-Binding Second Moment Approximation TBSMA potentials, [33] where the electron density of states in the region of an atom is calculated from a sum of contributions from surrounding atoms, and the potential energy contribution is then a function of this sum. Semi-empirical potentials[edit] Semi-empirical potentials make use of the matrix representation from quantum mechanics. However, the values of the matrix elements are found through empirical formulae that estimate the degree of overlap of specific atomic orbitals. The matrix is then diagonalized to determine the occupancy of the different atomic orbitals, and empirical formulae are used once again to determine the energy contributions of the orbitals. There are a wide variety of semi-empirical potentials, termed tight-binding potentials, which vary according to the atoms being modeled. Force field Most classical force fields implicitly include the effect of polarizability , e. These partial charges are stationary with respect to the mass of the atom. But molecular dynamics simulations can explicitly model polarizability with the introduction of induced dipoles through different methods, such as Drude particles or fluctuating charges. This allows for a dynamic redistribution of charge between atoms which responds to the local chemical environment. For many years, polarizable MD simulations have been touted as the next generation. For homogenous liquids such as water, increased accuracy has been achieved through the inclusion of polarizability. Quantum chemistry and List of quantum chemistry and solid state physics software In classical molecular dynamics, one potential energy surface usually the ground state is represented in the force field. This is a consequence of the Bornâ€”Oppenheimer approximation. In excited states, chemical reactions or when a more accurate representation is needed, electronic behavior can be obtained from first principles by using a quantum mechanical method, such as density functional theory. Due to the cost of treating the electronic degrees of freedom, the computational cost of these simulations is far higher than classical molecular dynamics. This implies that AIMD is limited to smaller systems and shorter times. Ab initio quantum mechanical and chemical methods may be used to calculate the potential energy of a system on the fly, as needed for conformations in a trajectory. This calculation is usually made in the close neighborhood of the reaction coordinate. Although various approximations may be used, these are based on theoretical considerations, not on empirical fitting. Ab initio calculations produce a vast amount of information that is not available from empirical methods, such as density of electronic states or other electronic properties. A significant advantage of using ab initio methods is the ability to study reactions that involve breaking or formation of covalent bonds, which correspond to multiple electronic states. A new class of method has emerged that combines the good points of QM accuracy and MM speed calculations. The cost of doing classical molecular dynamics MM in the most straightforward case scales O n2 , where n is the number of atoms in the system. This is mainly due to electrostatic interactions term every particle interacts with every other particle. In other words, if a system with twice as many atoms is simulated then it would take between two and four times as much computing power. To overcome the limit, a small part of the system is treated quantum-mechanically typically active-site of an enzyme and the remaining system is treated classically. This allows generating hydrogen wave-functions similar to electronic wave-functions. This methodology has been useful in investigating phenomena such as hydrogen tunneling. In this case, quantum tunneling is important for the hydrogen, as it determines the reaction rate. Instead of explicitly representing every atom of the system, one uses "pseudo-atoms" to represent groups of atoms. MD simulations on very large systems may require such large computer resources that they cannot easily be studied by traditional all-atom methods. Similarly, simulations of processes on long timescales beyond about 1 microsecond are prohibitively expensive, because they require so many time steps. In these cases, one can sometimes tackle the problem by using reduced representations, which are also called coarse-grained models. Such united atom approximations have been used in MD simulations of biological membranes. Implementation of such approach on systems where electrical properties are of interest can be challenging owing to the difficulty of using a proper charge distribution on the pseudo-atoms. The parameterization of these very coarse-grained models must be done empirically, by matching the behavior of the model to appropriate experimental data or all-atom simulations. Ideally, these parameters should account for both enthalpic and entropic contributions to free energy in an implicit way. When coarse-graining is done at higher levels, the accuracy of the dynamic description may be less reliable. But very coarse-grained models have been used successfully to examine a wide range of questions in structural biology, liquid crystal organization, and polymer glasses. Examples of applications of coarse-graining: Virtual cell simulation to study the interaction of cells and various substrates [46]. The simplest form of coarse-graining is the united atom sometimes called extended atom and was used in most early MD simulations of proteins, lipids, and nucleic acids. For example, instead of treating all four atoms of a CH3 methyl group explicitly or all three atoms of CH2 methylene group , one represents the whole group with one pseudo-atom. It must, of course, be properly parameterized so that its van der Waals interactions with other groups have the proper distance-dependence. Similar considerations apply to the bonds, angles, and torsions in which the pseudo-atom participates. In this kind of united atom representation, one typically eliminates all explicit hydrogen atoms except those that have the capability to participate in hydrogen bonds polar hydrogens. The polar hydrogens are usually retained in the model, because proper treatment of hydrogen bonds requires a reasonably accurate description of the directionality and the electrostatic interactions between the donor and acceptor groups. A hydroxyl group, for example, can be both a hydrogen bond donor, and a hydrogen bond acceptor, and it would be impossible to treat this with one OH pseudo-atom. About half the atoms in a protein or nucleic acid are non-polar hydrogens, so the use of united atoms can provide a substantial savings in computer time. Incorporating solvent effects[edit] In many simulations of a solute-solvent system the main focus is on the behavior of the solute with little interest of the solvent behavior particularly in those solvent molecules residing in regions far from the solute molecule. The use of non-rectangular periodic boundary conditions, stochastic boundaries and solvent shells can all help reduce the number of solvent molecules required and enable a larger proportion of the computing time to be spent instead on simulating the solute. It is also possible to incorporate the effects of a solvent without needing any explicit solvent molecules present. One example of this approach is to use a potential mean force PMF which describes how the free energy changes as a particular coordinate is varied. The free energy change described by PMF contains the averaged effects of the solvent. Long-range forces[edit] A long range interaction is an interaction in which the spatial interaction falls off no faster than r.

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