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*Incorporating quantum mechanics into an  
atomistic simulation necessarily involves*

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*solving the Schroedinger equation.*

*Unfortunately, the computational expense associated with solving this equation scales miserably with the number of included quantum degrees of freedom (DOF). The situation is so dire, in fact, that a molecular dynamics (MD) simulation cannot include more than a*

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*small number of quantum DOFs before it becomes computationally intractable.*

*Thus, if one were to simulate a relatively large system, such as one containing several hundred atoms or molecules, it would be unreasonable to attempt to include the effects of all of the electrons associated with all of the components of*

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*the system. The mixed quantum/classical (MQC) approach provides a way to circumvent this issue. It involves treating the vast majority of the system classically, which incurs minimal computational expense, and reserves the consideration of quantum mechanical effects for only the few degrees of freedom more directly*

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*involved in the chemical phenomenon being studied. For example, if one were to study the bonding of a single diatomic molecule in the gas phase, one could employ a MQC approach by treating the nuclei of the molecule's two atoms classically--including the deeply bound, low-energy electrons that change*

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*relatively little--and solving the Schroedinger equation only for the high energy electron(s) directly involved in the bonding of the classical cores. In such a way, one could study the bonding of this molecule in a rigorous fashion while treating only the directly related degrees of freedom quantum mechanically.*

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*Pseudopotentials are then responsible for dictating the interactions between the quantum and classical degrees of freedom. As these potentials are the sole link between the quantum and classical DOFs, their proper development is of the utmost importance. This Thesis is concerned primarily with my work on the*

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*development of novel, rigorous and dynamical pseudopotentials for use in mixed quantum/ classical simulations in the condensed phase. The pseudopotentials discussed within are constructed in an ab initio fashion, without the introduction of any empiricism, and are able to exactly reproduce the results of higher level, fully*



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*quantum mechanical Hartree-Fock calculations. A recurring theme in the following pages is overcoming the so-called frozen core approximation (FCA). This essentially comes down to creating pseudopotentials that are able to respond in some way to the local molecular environment in a rigorous fashion. The*

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*various methods and discussions that are part of this document are presented in the context of two particular systems. The first is the sodium dimer cation molecule, which serves as a proof of concept for the development of coordinate-dependent pseudopotentials and is the subject of Chapters 2 and 3. Next, the hydrated*

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*electron & mdash;the excess electron in liquid--water is tackled in an effort to address the recent controversy concerning its true structure and is the subject of Chapters 4 and 5. In essence, the work in this Dissertation is concerned with finding new ways to overcome the problem of a lack of infinite computer*

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*processing power.*

*This multi-author contributed volume includes methodological advances and original applications to actual chemical or biochemical phenomena which were not possible before the increased sophistication of modern computers. The chapters contain detailed reviews of the*

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*developments of various computational techniques, used to study complex molecular systems such as molecular liquids and solutions (particularly aqueous solutions), liquid-gas, solid-gas interphase and biomacromolecular systems. Quantum modeling of complex molecular systems is a useful resource for*

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*help the authors produce chapters that are complete, accurate, clear, and accessible to experimentalists (in particular) and other nonspecialists (in general)."*—**JOURNAL OF THE AMERICAN CHEMICAL SOCIETY**  
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and lists new techniques for classical MD • Deals with complex systems: biomolecules, aqueous solutions, ice and clathrates, liquid crystals, polymers •



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reactions, interfaces,  
catalysis, surface  
phenomena and solids  
Although the book is not  
formally divided into  
methods and applications,

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the chapters are arranged starting with those that discuss new algorithms, methods and techniques, followed by several important applications. This book provides a

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relatively complete  
introduction to the  
methods used in  
computational condensed  
matter. A wide range of  
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including traditional quantum chemistry methods, density functional theory, many-body perturbation theory, and more.

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discussed, with extensions to enhanced sampling and free-energy calculation techniques including umbrella sampling, metadynamics, integrated tempering sampling, etc.

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As a further extension beyond the standard Born-Oppenheimer molecular dynamics, some simulation techniques for the description of quantum nuclear effects are also

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covered, based on Feynman's path-integral representation of quantum mechanics. The book aims to help beginning graduate students to set up a framework of the concepts

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they should know before  
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explanation of the path-  
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taken in developing  
methodologies that can

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simulation of the metal cluster  $\text{Li}_6$  running on the Intel Touchstone Delta at Caltech.

A set of interatomic potentials for hydrocarbons that are based upon the self-consistent charge transfer tight-binding approximation to density functional theory have been developed

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and implemented into the quantum molecular dynamics code "LATTE". The interatomic potentials exhibit an outstanding level of transferability and have been applied in molecular dynamics simulations of tert-butylacetylene under thermodynamic conditions that correspond to its single-

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shock Hugoniot. We have achieved precise conservation of the total energy during microcanonical molecular dynamics trajectories under incomplete convergence via the extended Lagrangian Born-Oppenheimer molecular dynamics formalism. In good agreement with the results of a series of

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flyer-plate impact experiments, our SCC-TB molecular dynamics simulations show that tert-butylactylene molecules polymerize at shock pressures around 6.1 GPa.

The QM/MM method, short for quantum mechanical/molecular mechanical, is a highly versatile

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approach for the study of chemical phenomena, combining the accuracy of quantum chemistry to describe the region of interest with the efficiency of molecular mechanical potentials to represent the remaining part of the system. Originally conceived in the 1970s by the influential work of the the



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Nobel laureates Martin Karplus, Michael Levitt and Arieh Warshel, QM/MM techniques have evolved into one of the most accurate and general approaches to investigate the properties of chemical systems via computational methods. Whereas the first applications have been focused on studies of organic

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and biomolecular systems, a large variety of QM/MM implementations have been developed over the last decades, extending the range of applicability to address research questions relevant for both solution and solid-state chemistry as well. Despite approaching their 50th anniversary in

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2022, the formulation of improved QM/MM methods is still an active field of research, with the aim to (i) extend the applicability to address an even broader range of research questions in chemistry and related disciplines, and (ii) further push the accuracy achieved in the QM/MM description beyond that

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of established formulations. While being a highly successful approach on its own, the combination of the QM/MM strategy with other established theoretical techniques greatly extends the capabilities of the computational approaches. For instance the integration of a suitable QM/MM

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technique into the highly successful Monte-Carlo and molecular dynamics simulation protocols enables the description of the chemical systems on the basis of an ensemble that is in part constructed on a quantum-mechanical basis. This eBook presents the contributions of a recent Research

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Topic published in Frontiers in Chemistry, that highlight novel approaches as well as advanced applications of QM/MM method to a broad variety of targets. In total 2 review articles and 10 original research contributions from 48 authors are presented, covering 12 different

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countries on four continents. The range of research questions addressed by the individual contributions provide a lucid overview on the versatility of the QM/MM method, and demonstrate the general applicability and accuracy that can be achieved for different problems in chemical sciences. Together with the

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development of improved algorithms to enhance the capabilities of quantum chemical methods and the continuous advancement in the capacities of computational resources, it can be expected that the impact of QM/MM methods in chemical sciences will be further increased already in the near



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future.

New Developments in Quantum  
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The school held at Villa  
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July 1997 was very much an  
educational experiment aimed  
not just at teaching a new*

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*generation of students the latest developments in computer simulation methods and theory, but also at bringing together researchers from the condensed matter computer simulation community, the*

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*biophysical chemistry  
community and the quantum  
dynamics community to  
confront the shared problem:  
the development of methods  
to treat the dynamics of  
quantum condensed phase  
systems. This volume*

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*collects the lectures delivered there. Due to the focus of the school, the contributions divide along natural lines into two broad groups: (1) the most sophisticated forms of the art of computer simulation,*

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*including biased phase space sampling schemes, methods which address the multiplicity of time scales in condensed phase problems, and static equilibrium methods for treating quantum systems; (2) the*

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*contributions on quantum  
dynamics, including methods  
for mixing quantum and  
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*"Using the laws of quantum mechanics, it is possible to simulate the time evolution of molecular systems. The results of these simulations are of great importance to fields such as combustion, materials science, and drug*

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*design. They can be used to determine chemical properties such as critical points and reaction rates. However, the dimension of the Hilbert space that describes the wave function of a molecule scales*

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*exponentially with the size of the system. A solution to this scaling problem is to use quantum computers to simulate molecules. In this thesis, a strategy for conducting molecular dynamics simulations is*

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*explained in detail. This strategy involves using a hybrid algorithm known as the variational quantum eigensolver (VQE). The algorithm takes advantage of the computational power of both classical and quantum*

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*computers. It works by varying optimization parameters associated with the electronic wave function until the total electronic energy is minimized. Born-Oppenheimer molecular dynamics is then employed to*

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*determine the motion of the nuclei based on the results of the VQE. This method was tested by simulating the time evolution of H<sub>2</sub> using a quantum computer simulator. Attempts were also made to repeat this simulation with*

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*a superconducting quantum computer. Additionally, techniques to improve the efficiency of the VQE and the BOMD method are presented in this thesis. The first strategy consists in varying the number of*

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*quantum measurements during  
the VQE's optimization  
procedure. It was  
demonstrated that the number  
of measurements needed could  
be reduced by a factor of  
almost 3 for H2 by varying  
the number of measurements*



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*based on an exponential relationship. It was also shown that the initial guess for the optimization parameters could be improved during a BOMD simulation by utilizing results from previous time points. The*

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*average relative difference between the guessed parameters and the optimal ones was 2.5% when using a linear extrapolation technique to simulate the time evolution of H<sub>2</sub> . On the other hand, it was 35%*

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*when employing perturbation  
theory to generate  
guesses"--*

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**Addressing the need of chemistry,**

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photochemistry, reactive scattering, optical spectroscopy, or femto- and attosecond chemistry and spectroscopy underline that nuclear quantum mechanical effects affect many areas of chemical and physical research. In contrast to standard



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quantum chemistry calculations, where the nuclei are treated classically, molecular quantum dynamics can cover quantum mechanical effects in their motion. Many examples, ranging from fundamental to applied problems,

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are known today that are impacted by nuclear quantum mechanical effects, including phenomena like tunneling, zero point energy effects, or non-adiabatic transitions. Being important to correctly understand many observations in chemical,

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organic and biological systems, or for the understanding of molecular spectroscopy, the range of applications covered in this book comprises broad areas of science: from astrophysics and the physics and chemistry of the atmosphere,

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over elementary processes in chemistry, to biological processes (such as the first steps of photosynthesis or vision).

Nevertheless, many researchers refrain from entering this domain.

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Dynamics" offers them an accessible introduction. Although the calculation of large systems still presents a challenge - despite the considerable power of modern computers - new strategies have been developed to extend the studies to

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systems of increasing size. Such strategies are presented after a brief overview of the historical background. Strong emphasis is put on an educational presentation of the fundamental concepts, so that the reader can inform himself about the

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most important concepts, like eigenstates, wave packets, quantum mechanical resonances, entanglement, etc. The chosen examples highlight that high-level experiments and theory need to work closely together. This book thus is a

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must-read both for researchers working experimentally or theoretically in the concerned fields, and generally for anyone interested in the exciting world of molecular quantum dynamics.

Simulations as Data. Quantum

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Molecular Dynamics Contribution

Molecular Simulations

Parallelization of quantum molecular  
dynamics simulation code

experiments, theories and

simulations : meeting of the

European and Japanese Molecular

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liquid groups (EMLG/JMLG)

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Extended Lagrangian Quantum  
Molecular Dynamics Simulations of  
Shock-induced Chemistry in

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determine the forces quantum mechanically from density functional, extended Huckel, and tight binding techniques and move the nuclei according to the classical equations of motion. We determine pair-correlation

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functions, diffusion coefficients, and electrical conductivities. We find that many-body effects predominate in this regime. We begin to obtain agreement with the OCP and Thomas-Fermi models only at the higher

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manner and non-mathematical style, allowing students and researchers to access computational methods outside their immediate area of expertise. This thesis details both the technical and theoretical aspects

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of performing path integrals through classical Molecular Dynamics (MD) simulations. In particular, Graphics Processing Unit (GPU) computing is used to augment the Path Integral Molecular Dynamics (PIMD)

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portion of the widely available  
Molecular Modelling Tool Kit  
(MMTK) library. This same PIMD  
code is also extended in a  
different direction: a novel  
method for nuclear ground state  
property prediction is introduced

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that closely mimics existing code in functional form. In order to add GPU computing capabilities to the existing MMTK codebase, the open source Open Molecular Mechanics (OpenMM) library was used. OpenMM provides

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high performance

implementations of a variety of commonly used MD algorithms, with the goal of supporting current and future specialized hardware. Due to the object oriented nature of both codes,

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and the use of SI units in each, the development process was rather painless. The integration of OpenMM with MMTK is seamless, and arbitrary systems are supported without the user even needing to know that GPU

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acceleration is being used. The hybrid OpenMM-MMTK code is benchmarked against the vanilla MMTK code in terms of speed and accuracy, and the results show that GPU computing is the obvious choice for PIMD

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simulations. Starting with a desire to apply the highly efficient Path Integral Langevin Equation (PILE) thermostat to the Path Integral Ground State (PIGS) problem, a new hybrid PILE-PIGS, or LE-PIGS, method



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was developed. This thesis describes the theoretical justification for this method, including the introduction of a modified normal mode representation based on the Discrete Cosine Transform

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(DCT). It is shown that in DCT space, the equations of motion of a PIGS system are virtually identical to the equations of motion of a PIMD system in Fourier space. This leads to direct reuse of existing PILE

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code in MMTK, and options to extend this ground state problem to OpenMM for the purpose of GPU acceleration. The method is applied to a series of model systems, and in each case convergence to the exact ground

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with a Quantum-chemical Core  
Quantum Molecular Dynamics  
Simulations of Processes in  
Large Clusters  
Approximations, Algorithms,  
Implementation and Applications

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Path Integral Approaches and  
Graphics Processing Unit Tools  
for Quantum Molecular  
Dynamics Simulations

Les résultats de nos  
simulations sont en très  
bon accord avec les

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expériences. De plus,  
nos calculs fournissent  
une caractérisation  
détaillée des processus  
microscopiques  
apparaissant pendant la  
collision.

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Constant-volume quantum molecular dynamics (QMD) simulations of uranium (U) have been carried out over a range of pressures and temperatures that span



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the experimentally  
observed solid  
orthorhombic [alpha]-U,  
body-centered cubic  
(bcc), and liquid  
phases, using an ab  
initio plane-wave

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pseudopotential method within the generalized gradient approximation of density functional theory. A robust U pseudopotential has been constructed for these

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simulations that treats the 14 valence and outer-core electrons per atom necessary to calculate accurate structural and thermodynamic properties up to 100 GPa. Its

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validity has been checked by comparing low-temperature results with experimental data and all-electron full-potential linear-muffin-tin-orbital calculations

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of several different  
uranium solid  
structures. Calculated  
QMD energies and  
pressures for the  
equation of state of  
uranium in the solid and

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liquid phases are given,  
along with results for  
the Grueneisen parameter  
and the specific heat.  
We also present results  
for the radial  
distribution function,

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bond-angle distribution function, electronic density of states, and liquid diffusion coefficient, as well as evidence for short-range order in the liquid.

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Free energy calculations are one of the most powerful tools within modern theoretical chemistry and are often used to make comparisons with experimental



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results. Existing free energy calculations are typically performed for classical molecular dynamics simulations but there are certain systems where nuclear

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quantum effects play an integral role.

Specifically, systems with light atoms or low temperatures are the most influenced by such nuclear quantum effects

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and the development of Feynman path integrals [1] has been effective in accurately describing the quantum nature of these nuclei [2-8]. The primary objective of

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this thesis is the  
development of a pair of  
methodologies to  
calculate free energies  
utilizing path integral  
molecular dynamics to  
account for nuclear

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quantum effects. Prior to the development of these free energy methodologies, this thesis presents a communication interface between the OpenMM and

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MMTK software packages that has been previously published [9]. This interface allows for users of MMTK to take advantage of the performance of OpenMM

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without major modifications to existing simulation scripts. Notably, the serial OpenMM integrator is shown to provide a 3x performance gain in

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comparison to a standard  
MMTK simulation while  
the GPU implementations  
of OpenMM provide over a  
400x performance gain  
for larger systems with  
periodic boundary



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conditions. The first path integral free energy methodology of this thesis combines the existing umbrella sampling technique [10,11] with path

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integral molecular  
dynamics. This  
methodology has been  
previously published and  
proposes that the  
umbrella sampling  
biasing potential only

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needs to be applied to a single path integral bead [12]. Furthermore, this proposed methodology is successfully benchmarked for a pair of Lennard-

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Jones dimer systems before being applied to the more difficult water dimer. The free energy profiles obtained from simulation are then used to calculate a free

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energy difference of  
 $-12.90 \pm 0.05$  kJ/mol for  
the MB-Pol potential in  
comparison to the  
experimental  
dissociation energy of  
 $-13.2 \pm 0.12$  kJ/mol

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[13]. The second path integral free energy methodology introduces a constraint within the path integral molecular dynamics simulations as opposed to an umbrella

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sampling restraint.

Specifically, this methodology applies a constraint to an individual path integral bead in a manner that is similar to the concept

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of thermodynamic  
integration for  
classical simulations  
[14]. Formal estimators  
for the derivative of  
the free energy have  
been developed by



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Iouchtchenko et al. [15]  
and the results  
presented in this thesis  
analyze the  
effectiveness of these  
estimators for molecular  
dynamics simulations of

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Lennard-Jones and water dimers. Additionally, a new estimator is developed and the resulting free energy profiles are used to evaluate a free energy

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difference for the water dimer of  $-13.03 \pm 0.14$  kJ/mol, which is within the errors of the experimental dissociation energy [13]. Overall, this

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thesis provides a theoretical framework to study the free energy of weakly bound systems over a broad range of temperatures. It is important to note that

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these methodologies were insufficient below 25 K and it remains more practical to use reaction coordinates that are not distances at such temperatures.

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Nevertheless, the extension and application of these methodologies to more complicated systems remains an area of exciting development.

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Quantum Molecular  
Dynamics Simulations of  
Materials  
Tight-binding Quantum  
Molecular Dynamics  
Simulations of Hydrogen  
in Silicon

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Methods and Applications  
Simulations as Data  
Methodology and  
Applications in  
Photochemistry and  
Bioinorganic Chemistry  
Multiscale Dynamics



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We are using classical molecular dynamics and condensed phase electronic-structure methods to predict some of the thermophysical and mechanical properties that are needed as

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input to realistic mesoscale models for plastic-bonded explosives. The main materials studied to date are HMX, PETN, Estane copolymer, and bi(2,2-dinitropropyl) formal/acetal (BDNPF/A).

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Emphasis is placed on non-reactive properties and thermodynamic states relevant to cookoff and shock initiation phenomena. Both crystal and liquid-state properties are of interest. Typical simulation sizes

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and times are (almost equal to) 102 molecules and 2-10 ns, respectively. The overarching goal is to develop internally consistent model thermodynamic and elastic mechanical descriptions for the

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materials. Prioritization among the set of properties amenable to atomistic simulation is made based on ongoing interactions with mesoscale modelers at Los Alamos and elsewhere. Recent work will be summarized and

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our view of profitable directions for future research will be discussed, including preliminary results for large-scale molecular dynamics simulations of shock response of crystalline HMX. Reviews in Computational

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The Development of Rigorously  
Correct, Dynamical  
Pseudopotentials for Use in  
Mixed Quantum/classical  
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in the Condensed Phase

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Molecular Systems  
Molecular Dynamics  
Quantum Mechanical  
Development of Potential  
Energy Parameters for  
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of the Clay/solution Interface  
TREEQMD