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**Oku, K., M. Kurose, M. Kubota, S. Fukuda, M. Kurimoto, Y. Tujisaka, A. Okabe, and M. Sakurai (2005).** "Combined NMR and Quantum Chemical Studies on the Interaction between Trehalose and**


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This paper presents the results obtained using a genetic algorithm (GA) to search for stable structures of medium size silicon clusters. In this work the GA uses a semiempirical energy function to find the best cluster structures, which are further optimized using density-functional theory. For small clusters our results agree well with previously reported structures, but for larger ones different structures appear. This is the case of Si36 where we report a different structure, with significant lower energy than those previously found using limited search approaches on common structural motifs. This demonstrates the need for global optimization schemes when searching for stable structures of medium-size silicon clusters. ©2004 The American Physical Society.


Although electrons having enough energy to ionize or electronically excite DNA have long been known to cause strand breaks (i.e., bond cleavages), only recently has it been suggested that even lower-energy electrons (most recently 1 eV and below) can also damage DNA. The findings of the present work suggest that, while DNA bases can attach electrons having kinetic energies in the 1 eV range and subsequently undergo phosphate-sugar O-C bond cleavage, it is highly unlikely (in contrast to recent suggestions) that electrons having kinetic energies near 0 eV can attach to the phosphate unit's P=O bonds. Electron kinetic energies in the 2-3 eV range are required to attach directly to DNA's phosphate group's P=O * orbital and induce phosphate-sugar O-C bond cleavages if the phosphate groups are rendered neutral (e.g., by nearby counterions). Moreover, significant activation barriers to C-O bond breakage render the rates of both such damage mechanisms (i.e., P=O-attached and base-attached) slow as compared to electron autodetachment and to other damage processes.


This paper presents a comparison of the embedded ion method (EIM) and the surface charge representation of the electrostatic embedding potential (SCEEP) method, two methods which can be used to calculate solid-state effects on NMR chemical shifts. The results in a selected group of compounds with known solid-state NMR data and neutron diffraction structures, confirm that these effects are important in both C and N chemical shifts. The solid-state effects calculated by both methods are similar and of equal statistical quality when compared with the experimental data. Iterative schemes to calculate, in a self-consistent fashion, the charges used to simulate the crystalline field are very important for ionic compounds.


The skill of a mesoscale-model-based model output statistics (MOS) system that provided hourly forecasts for 18 sites over northern Utah during the 2002 Winter Olympic and Paralympic Games is evaluated. The MOS system was developed using three winters (November-April 1998/99, 1999/2000, and 2000/01) of forecasts by the fifth-generation Pennsylvania State University-National Center for Atmospheric Research Mesoscale Model (MM5) and observations from Olympic venues and transportation corridors. MOS temperature, relative humidity, wind speed, and wind direction forecasts were considerably more accurate than those produced by the 12- and 4-km MM5 grids. A primary contributor to MM5 temperature and relative humidity errors was a systematic overprediction of surface temperature (i.e., a warm/dry bias) during persistent and nocturnal cold-pool events when corresponding errors in MM5 dewpoint temperature forecasts
were not observed. MOS largely corrected for this temperature bias. MOS wind speed forecasts outperformed the 12- and 4-km MM5 forecasts by the largest margin at locations with the lowest wind speed variability. Raw model and MOS performance exhibited minimal sensitivity to variations in model initial and lateral boundary conditions (derived from the forecasts of either the National Centers for Environmental Prediction's Eta Model or the Aviation run of the Global Spectral Model). MOS temperature, relative humidity, and wind speed forecasts were equal to or more skillful than human-generated forecasts produced by the Olympic Forecast Team. The results illustrate that statistical techniques continue to improve upon purely numerical predictions even at high resolution. This is particularly true in a region of complex terrain where detailed characteristics of local topography and microclimates remain unresolved. It is recommended that traditional MOS or other statistical techniques based on high-density surface observations available from the MesoWest cooperative networks be used to improve gridded forecast products created by the National Weather Service Interactive Forecast Preparation System (IFPS) and other applications.


A novel least-squares fitting approach is presented to obtain classical force fields from trajectory and force databases produced by ab initio (e.g., Car-Parrinello) molecular dynamics (MD) simulations. The method was applied to derive effective nonpolarizable three-site force fields for liquid water at ambient conditions from Car-Parrinello MD simulations in the Becke-Lee-Yang-Parr approximation to the electronic density functional theory. The force-matching procedure includes a fit of short-ranged nonbonded forces, bonded forces, and atomic partial charges. The various parameterizations of the water force field differ by an enforced smooth cut-off applied to the short-ranged interaction term. These were obtained by fitting to the trajectory and force data produced by Car-Parrinello MD simulations of systems of 32 and 64 H2O molecules. The new water force fields were developed assuming both flexible or rigid molecular geometry. The simulated structural and self-diffusion properties of liquid water using the fitted force fields are in close agreement with those observed in the underlying Car-Parrinello MD simulations. The resulting empirical models compare to experiment much better than many conventional simple point charge (SPC) models. The fitted potential is also shown to combine well with more sophisticated intramolecular potentials. Importantly, the computational cost of the new models is comparable to that for SPC-like potentials. ©2004 American Institute of Physics.


A semiclassical initial value representation (SC-IVR) for centroid dynamics (CD) is derived to provide a more accurate description of quantum time correlation functions (TCFs). The time-dependent quasi-density operator (QDO) in SC-IVR-CD is shown to exhibit more exact behavior than that of the CMD approximation, thereby improving the calculated quantum TCFs. Three typical one-dimensional model potentials (weak anharmonic, double well, and quartic) were studied as examples in calculating TCFs with the SC-IVR-CD method. Importantly, for intermediate temperatures, SC-IVR-CD gives a more exact description of the coherent behavior of the quantum TCFs than does centroid molecular dynamics (CMD).


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The modified genetic algorithm (MGAC) has been extended to allow simultaneous relaxation of molecular geometry during optimization of the crystalline structure. The method was applied to L-alanine and DL-alanine for two different potential functions. The genetic algorithm was always able to find minima that are likely global minima of the crystalline potential, showing good agreement with the experimental structures. For DL-alanine MGAC located the experimental crystalline structure but also consistently found a different low-energy crystalline structure that it is an excellent candidate for a polymorph. © 2003 Wiley Periodicals, Inc. Int J Quantum Chem, 2004


A lipid bilayer is modeled using a mesoscopic model designed to bridge atomistic bilayer simulations with macro-scale continuum-level simulation. Key material properties obtained from detailed atomistic-level simulations are used to parameterize the meso-scale model. The fundamental length and time scale of the meso-scale simulation are at least an order of magnitude beyond that used at the atomistic level. Dissipative particle dynamics cast in a new membrane formulation provides the simulation methodology. A meso-scale representation of a dimyristoylphosphatidylcholine membrane is examined in the high and low surface tension regimes. At high surface tensions, the calculated modulus is found to be slightly less than the atomistically determined value. This result agrees with the theoretical prediction that high-strain thermal undulations still persist, which have the effect of reducing the value of the atomistically determined modulus. Zero surface tension simulations indicate the presence of strong thermal undulatory modes, whereas the undulation spectrum and the calculated bending modulus are in excellent agreement with theoretical predictions and experiment.


This paper describes a new computational scheme to model crystal structures of organic compounds employing a modified genetic algorithm. The method uses real-valued Cartesian coordinates and Euler angles between molecules in a crystal block as variables identifying the genetic parameters, i.e., genes. The model does not make any assumption on the crystallographic group at which the compound belongs nor to the number of molecules in the unit cell.
cell. The method has been implemented in the computer package MGAC (Modified Genetic Algorithm for Crystal and Cluster structures) that allows for optimizations using any arbitrary selection function. The examples presented here for the crystalline structures of benzene, naphthalene and anthracene, using an empirical potential energy function as the selection function, show excellent agreement with the experimental ones. While these examples use the "rigid molecule approximation," the method is quite general and can be extended to take into account any number of intramolecular degrees of freedom. ©2002 American Institute of Physics.


This paper investigates the diurnal evolution of thermally driven plain-mountain winds, up- and down-valley winds, up- and downslope winds, and land-lake breezes for summer fair weather conditions in four regions of the Intermountain West where dense wind networks have been operated. Because of the diverse topography in these regions, the results are expected to be broadly representative of thermally driven wind climates in the Intermountain West. The regions include the Wasatch Front Valleys of northern Utah, the Snake River Plain of Idaho, the southern Nevada basin and range province, and central Arizona. The analysis examines wind characteristics, including the regularity of the winds and interactions of the four types of thermally driven winds, using meteorological data from the University of Utah's MesoWest network. In general, on fair weather days, winds in all four regions exhibit a consistent direction from day to day at a given hour. A measure of this wind consistency is defined. The nighttime hours exhibit a generally higher consistency than the daytime hours. Lower consistency during the day-night and night-day transition periods reflects day-to-day variations in the timing of wind system reversals. Thermally driven circulations are similar in the four regions, but the Wasatch Front Valleys are influenced by lake breezes from the adjacent Great Salt Lake, the Snake River Plain is influenced by along-plain circulations and localized outflow from the Central Idaho Mountains, and winds in both southern Nevada and central Arizona are influenced by plain-mountain circulations associated with regionalscale contrasts in elevation and surface heating.


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