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14. ABSTRACT

This final report describes the efforts to develop computational-chemistry technology aimed at enabling simulation of gas/surface collisions of interest to the US Air Force that have been carried out under contract FA9550-06-1-0165. The report includes advances in three separate, but complementary lines of research that had the overarching goal of performing atomistic simulations of high-energy collisions between gases and surfaces with unprecedented levels of accuracy. These three lines are: 1) Development of specific-reaction-parameters semiempirical Hamiltonians for the study of the dynamics of radical+alkane reactions, 2) Classical-trajectory simulations of hyperthermal collisions between closed-shell Ar atoms and perfluorinated organics, and 3) Investigation of energy exchange in collisions of closed-shell gases with alkanethiolate self-assembled monolayers. The principal outcome of this project was the advancement of computational-chemistry techniques that can be used to simulate chemical reactions occurring on and around spacecraft in orbit with accuracy.

15. SUBJECT TERMS

Computational chemistry. Theoretical chemistry. Hyperthermal collisions. Gas/surface energy exchange. Reaction dynamics.

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Final Performance Report

Accurate characterization of the chemical reactions occurring on an around spacecraft in orbit is of importance for a better understanding of a variety of phenomena, including degradation of polymeric thermal insulators coating spacecraft and spectral signature of thruster plumes. This report describes the results of research developed under AFOSR support that has enhanced the tools available for theoretical study of the dynamics of large chemical reactions, in particular, gas/organic-surface reactions, with accuracy. The report contains an independent detailed description of each of the three main research thrusts that have benefitted from AFOSR support. A brief introduction is provided in each section, followed by an extensive account of the pertinent results. All of the results have been published, and full references to the publications are available at the end of the document. Overall, 13 peer-reviewed publications have emerged as a result of this work.

1) Development of low-cost electronic-structure methods for reaction-dynamics simulations of large chemical reactions

Despite significant progress in the development of analytic potential-energy surfaces (PES) for dynamics calculations of polyatomic chemical reactions, these functions remain difficult to derive. An alternative to deriving analytic PES for highly multidimensional problems, such as gas/organic-surface reactions, is to perform direct-dynamics simulations. In direct dynamics, the development of an analytic PES is entirely avoided by carrying out electronic-structure calculations whenever the forces acting on the nuclei (energy gradients) are needed during the dynamics simulation. An obvious issue with the direct-dynamics approach is that common reaction-dynamics studies involve calculation of literally tens of millions of energy gradients, particularly if the classical-trajectory method is used. Calculation of such a large number of energy derivatives using quantum-mechanical electronic-structure methods poses a tremendous constraint in the method and basis set used to solve the electronic Schrödinger equation. For instance, recent direct-dynamics studies on a reaction as simple as $H+CH_4$ (one heavy atom) could only calculate a relatively small number of trajectories with the modest

B3LYP/6-31G* method due to the computational expenditure associated with more accurate quantum-mechanical methods. Similarly, classical-trajectory calculations of the reactions of chlorine radicals with short-chain hydrocarbons were forced to start at the transition state due to the computational expenditure associated with propagating the equations of motion from reagents to products, even though the reactions included only two or three non-hydrogen atoms. Those examples showed that using low-level electronic-structure methods (such as Hartree-Fock) yields inaccurate dynamics results. This is not surprising, as the potential-energy surface governs the outcome of molecular collisions.

A significant portion of our efforts with AFOSR support has been directed at improving semiempirical Hamiltonians for reaction-dynamics calculations. Semiempirical Hamiltonians are derived from Hartree-Fock theory by neglecting and parametrizing some of the most computationally-expensive electronic integrals. These dramatic approximations, in addition to the use of pseudo-minimal basis sets, make these electronic-structure methods orders of magnitude faster than first-principles methods, but also very inaccurate. Therefore, even though the minimal computational requirements of semiempirical Hamiltonians afford dynamics studies of large systems, the general poor quality of these methods often yields wrong results. More than 15 years ago, Truhlar proposed an elegant approach to improve the accuracy of semiempirical Hamiltonians without compromising their speed. The approach was based on reoptimizing the semiempirical parameters contained in the Hamiltonian for a particular reaction, so that the Hamiltonian was accurate for that specific reaction. After this seminal paper, timid attempts by other authors to develop specific-reaction-parameters (SRP) Hamiltonians were focused on obtaining accurate descriptions of the potential-energy surface of specific reactions only along the minimum-energy path.

Since 2005, we have been working on deriving SRP semiempirical Hamiltonians that are accurate along not only the minimum-energy reaction path, but also elsewhere in the global potential-energy surface of a specific chemical reaction. Our investigations have targeted a variety of radical+methane reactions with very different potential-energy surface profiles. Our initial studies focused on the $O(^3P)+CH_4 \rightarrow OH+CH_3$ reaction. Using ab initio calculations of the global potential-energy surface as a reference, we produced a SRP Hamiltonian that furnished OH internal-state distributions in agreement with experiment for the first time. The results of our SRP Hamiltonian clearly improved over those of an analytical PES extant in the literature. Encouraged by this success, we proceeded to prove the generality of our approach by deriving SRP Hamiltonians for other important radical+methane reactions. The $F+CH_4 \rightarrow HF+CH_3$ reaction is poised to become a benchmark in the field of polyatomic reaction dynamics due to the availability of a wealth of experimental information on HF rovibrational-state distributions, angular distributions, state-specific excitation functions, and reactive resonances at near-threshold energies. Using ab initio information at the CCSD(T) level, we derived a SRP PM3 Hamiltonian to investigate some of the interesting dynamics properties of this reaction. Subsequent classical-trajectory calculations provided HF rovibrational distributions and excitation function in agreement with experiments The results provided by the SRP PM3 Hamiltonian were superior to those obtained with prior analytical and interpolated potential-energy surfaces. We showed that the superior performance of our SRP Hamiltonian can be tied to its better description of high-quality ab initio information of the global potential-energy surface, compared with the analytical and interpolated PES. Additional SRP Hamiltonian development for the $Cl+CH_4 \rightarrow HCl+CH_3$ reaction, spurred interest in the experimental group of Orr-Ewing (Bristol University, UK). Current collaborative efforts with that group are targeting the development of SRP Hamiltonians for the $Cl+C_2H_6$ and $Cl+CH_3OH$ reactions.

AFOSR support since March 2006 enabled us to take an important step in the SRP-Hamiltonian development field toward our goal of investigating gas/organic-surface reactions. Our studies of the $Cl+CH_4 \rightarrow HCl+CH_3$ and $Cl+C_2H_6 \rightarrow HCl+C_2H_5$ reactions revealed an important limitation of our work: even though the reactions are quite similar, an SRP Hamiltonian needed to be derived for each specific chemical reaction under consideration. With AFOSR support, we have been able to explore whether reoptimized Hamiltonians can be developed for a *family* of chemical reactions, instead of only *one* specific reaction. Our work has focused on the H+alkane family of reactions, for which detailed experimental information exists. To derive a Hamiltonian that is accurate for H+alkane reactions, we performed high-accuracy ab initio calculations (CCSD(T) extrapolated to the complete basis-set limit) of the two smallest homologues of the family ($H+CH_4$ and $H+C_2H_6$). Using ab initio data of the global potential-energy surfaces of both reactions, we reoptimized the parameters of the MSINDO Hamiltonian so that the semiempirical energies matched as closely as possible the CCSD(T) estimates. The SRP-MSINDO Hamiltonian that we derived shows a better description of the potential-energy surfaces than MP2 and B3LYP methods with complete basis-set (CBS) extrapolation. For instance, the error in the reaction energies and barriers of those first-principle methods is about 5 kcal/mol. SRP-MSINDO shows deviations of only 1-2 kcal/mol with respect to CCSD(T)/CBS estimates for both $H+CH_4$ and $H+C_2H_6$. However, SRP-MSINDO is orders of magnitude faster than the first-principles methods and enables detailed dynamics studies that are in principle more accurate than MP2 or B3LYP direct-dynamics studies.

To prove the global accuracy of the SRP-MSINDO Hamiltonian, we performed quasiclassical-trajectory (QCT) calculations at the high energies, and compared with the available experimental information, and with the results of other available potential-energy surfaces. For instance, we computed CH_3 product speed distributions generated in the $H+CH_4 \rightarrow H_2+CH_3$ reaction at 1.52 eV collision energy (E_{coll}) and compared them with the experiments of the Zare group, and with the results yielded by the state-of-the-art ZBB3 PES of Bowman and co-workers. Both calculated results are in excellent agreement with experiment, denoting accuracy in the potential-energy surfaces. Additional comparisons in other dynamics properties (excitation functions and HD rovibrational distributions) show similar levels of agreement between the calculated results and experiment.

Two characteristics of the SRP-MSINDO Hamiltonian that we derived are noteworthy. First, the dynamics results it provides are of similar quality to those of the analytic ZBB3 PES. However, only 600 ab initio points were used to derive the SRP-

MSINDO Hamiltonian, while over 50,000 were needed in the development of the ZBB3 PES. Second, the SRP-MSINDO Hamiltonian is also valid for the H+ethane reaction because part of the 600 ab initio points employed in the parameter reoptimization corresponded to regions of the $H+C_2H_6$ potential-energy surface. On the other hand, the ZBB3 PES is specific to $H+CH_4$. To corroborate that the accuracy shown by the SRP-MSINDO Hamiltonian for the $H+CH_4$ reaction is maintained for $H+C_2H_6$, we computed the excitation function of the $H+C_2D_6 \rightarrow HD+C_2D_5$ reaction obtained via direct-dynamics with the SRP-MSINDO Hamiltonian and compared it with the experiments of Oldershaw and Gould. As in the $H+CH_4$ system, the agreement between the SRP-MSINDO and experiment was very good. We note that, to the best of our knowledge, these were the first detailed dynamics simulations on the $H+C_2D_6$ reaction that have reproduced experiments.

Once we verified that one can generate an accurate semiempirical Hamiltonian specific to the $H+CH_4$ and $H+C_2H_6$ reactions, we used the Hamiltonian to decipher the dynamics of H+alkane reactions, including the H+propane reaction. Comparative studies of the H+alkane family of reactions had been lacking due to the difficulty in deriving potential-energy surfaces for all of the reactions in the family. Therefore, our calculations are the first of this kind. Several important conclusions emerged from our comparative study. Investigation of how energy is released among the various product degrees of freedom in H+alkane $\rightarrow$ H_2+alkyl reactions revealed that most of the energy available to products is channeled into relative product translation. Significantly less energy goes into rotation and vibration of the newly-formed H_2 molecule or alkyl product. An interesting result is that the size of the alkane molecule from which H-abstraction is produced influences the amount of energy that the alkyl fragment receives during the reaction; larger alkane molecules are able to draw more energy into the corresponding alkyl products at the expense of product translation.

After characterizing the dynamics of the H+alkane family of reactions, we attempted a similar effort for the F+alkane family, which has been under intense scrutiny from experiment in recent time. Using a strategy analogous to that described before for the H+alkane family, we obtained a SRP-MSINDO Hamiltonian specific to the F+alkane → HF+alkyl group of reactions. Subsequent trajectory calculations employing the SRP-MSINDO method, yielded HF vibrational-energy distributions in agreement with experiment. Other calculated trends were also in agreement with experiment, including the evolution of HF vibrational and rotational energy, and product relative translation with collision energy, and the evolution of the angular distributions for various HF(v') states. This last point is especially important, because experiment inferred that the evolution from backward to forward scattering for HF with increasing levels of vibrational excitation was a quantum-dynamics phenomenon. Our purely classical trajectories showed that the trend seen in the experiment does not require quantum-dynamical behavior. Instead, trajectories that produce reaction at large impact parameter tend to form highly-vibrationally excited HF, which scatters forwards. Additional results shed light on the dependence of the dynamics of the reaction on the size of the alkane molecule. Much as in the H+alkanes reactions, our scattering calculations indicate that the portion of energy received by the alkyl product increases with the size of the parent alkane reactant. In addition, we were able to identify the different dynamics of primary vs secondary vs tertiary abstraction sites. For instance, the calculations reveal that abstraction at tertiary sites produces more backward angular distributions than at primary sites, because reactions at primary sites are more peripheral than at tertiary sites.

2) Characterization of gas/organic-surface energy exchange at superthermal energies (0.1-1.0 eV)

Investigation of inelastic energy exchange in gas/surface processes is of chief importance, as these studies elucidate whether the gas tends to accommodate on the surface or recoils impulsively regardless of reaction. The Nathanson group has pioneered studies of gas/organic-surface energy exchange using closed-shell gases and hydrocarbon liquids. Recent experimental work in this field has favored use of alkanethiol self-assembled monolayers (SAMs) as the organic substrate because these structures afford precise control over the chemical and physical properties of the surface that is not possible using liquids. These attractive characteristics of SAMs have triggered substantial experimental studies of gas/surface energy exchange, which have primarily involved rare gases as the impinging gas species. Theory has proved invaluable in understanding the details of rare-gas/SAM inelastic collisions, with the trajectory calculations conducted by the Hase group playing a leading role.

Since 2005, our work in the gas/surface energy-exchange field has been focused on determining the level of accuracy required in the gas/surface potential-energy surface to obtain predictive results, and understanding the effect of the SAM density on the dynamics of gas/surface collisions. With AFOSR support, we embarked on new avenues in this field as part of a collaborative effort with the molecular-beam scattering group of Morris at Virginia Tech. A particularly longstanding issue in this field that we sought to address was the role played by surface mass in the dynamics of interfacial energy exchange. The work by the Nathanson group on gas/liquid scattering was not able to unequivocally resolve the effect of surface mass on the dynamics of gas/surface scattering. The problem encountered in those experiments is that to change the mass of the liquid surfaces beyond isotopic substitution, one necessarily needs to use liquids with different chemical groups (e.g. squalane and perfluoropolyether). Unfortunately, different liquids have different surface structure, which also affects energy transfer and inhibits elucidation of the role played solely by surface mass on energy transfer. A similar predicament has affected recent work by the Nesbitt group on the scattering of CO_2 from various organic liquids.

Our recently-published joint theory-experiment work using self-assembled monolayers (SAMs) has permitted us to separate for the first time the effect of surface mass on gas/organic-surface energy transfer from structural effects. To achieve this goal, we scattered Ne, Ar, and Kr from regular (CH_3-terminated) and ω-fluorinated (CF_3-terminated) alkanethiolate SAMs on Au(111). Note that the CH_3- and CF_3-terminated surfaces have the same structure, but different terminal groups, and therefore different surface mass. The results of our trajectory calculations reproduce well the molecular-beam scattering results obtained in the Morris lab: while the energy exchange in collisions with 0.6 eV Ne is very sensitive to whether the SAM terminus is a CH_3- or a

CF_3- group, 0.6 eV Kr is essentially insensitive to that difference. Extensive ab initio calculations indicated that the rare-gas/surface potentials for both SAMs are very similar, so the different scattering dynamics for the two surfaces are mostly a result of the different mass of the terminal group in the SAMs.

The result that surface mass controls the difference in the scattering from CH_3 and CF_3-SAM surfaces at the initial conditions of the molecular-beam experiments of the Morris group was nicely corroborated by comparison of the results of Ne/SAM trajectory calculations for a CH_3-terminated SAM, a CF_3-terminated SAM, and a CH_3-terminated SAM in which the three H atoms of the CH_3 terminus have a mass of 19.0 amu (F mass). All the terms of the CH_3-SAM potential energy surface were unchanged in this isotopic calculation. The calculations revealed that the surface mass change when going from CH_3- to CF_3-SAMs fully explains the difference in the energy transferred to these surfaces in Ne collisions.

The fact that kinematic factors control the difference in the scattering of 0.6 eV Ne, Ar, and Kr from CH_3- and CF_3-SAM permitted us to shed light on the experimental results. Optimum gas-to-SAM energy transfer requires the chains to move laterally to dissipate energy. The larger mass of CF_3-SAMs imparts an inertial barrier to lateral motion that is larger than in the case of CH_3-SAMs, so in principle, energy transfer to the heavier SAMs should be smaller. 0.6 eV Ne does not have enough momentum to displace the CF_3-SAM chains as much as it does the CH_3-SAM chains, and therefore cannot transfer as much energy to the heavier SAM. The larger momentum of 0.6 eV Ar enhances the lateral motion of the CF_3-SAM chains, but differences with the CH_3-SAM still persist. The momentum of 0.6 eV Kr is so large that the increased inertial barrier of the heavier SAM cannot be appreciated.

This work required an extensive study of the potential-energy surfaces of rare gases interacting with alkanes and fluoroalkanes, which was also carried out with AFOSR support. An important point in that publication was our demonstration that the focal-point approximation works superbly for dispersion interactions acting between rare gases and alkane molecules. This approximation enables the estimation of CCSD(T) energies from MP2 calculations with average errors in the global intermolecular potential-energy surface below 0.05 kcal/mol. The average errors in the long-range attractive well of the potential-energy surface are below 0.01 kcal/mol. These results are important, as the focal-point approximation offers a factor of 60 (!) decrease in computational time for systems as small as Ar—CF_4 . (The time savings for systems with more electrons are even larger.) The fascinating performance of the focal-point approximation for rare gas/closed-shell molecule interacting pairs put forward in our paper is making an impact in the field, and other researchers are starting to use it for similar problems.

A significant step forward in our understanding of gas/surface energy exchange was given via study of collisions of CO with SAMs. In contradistinction to our work on rare gases, the presence of rotational and vibrational degrees of freedom in CO enabled us to probe the involvement of the gas internal motions in gas/surface energy transfer. The results of our gas/surface classical-trajectory calculations agreed quite well with the molecular-beam experiments carried out in the Morris group, therefore, we further analyzed the calculations to learn aspects of the scattering process not directly available from experiment. In particular, we learned that the collisions are entirely vibrationally adiabatic, and CO rotation is only weakly coupled to the energy-transfer coordinate. Furthermore, if CO collides with the organic surfaces having a large amount of rotational energy before impact, the surfaces act as an effective sink of CO rotational excitation. Additional insight into gas/surface energy-exchange phenomenology was obtained from a thorough analysis of the collisions stereodynamics. In particular, we interrogated the orientation and alignment of the CO molecule's rotational angular momentum with respect to various axes of reference to determine the type of rotational motion that CO possesses after collision with the SAMs. Interestingly, we found that in addition to the expected cartwheel topspin motion, corkscrew or propeller motion, in which the CO molecule is rotating in a plane perpendicular to the direction of travel, is a favored rotational motion after collision. This intriguing result deviates from the results obtained before using metal surfaces and indicates the wealth of phenomena experienced when gases scatter from organic surfaces.

3) Study of inelastic energy transfer in extreme environments (5-15 eV collision energy)

AFOSR support since March 2006 has enabled us to augment our understanding of collision-induced dissociation of organic molecules by high-energy closed-shell species. Specifically, we investigated collisions of C_2H_6 and C_2F_6 with hyperthermal Ar (6-12 eV). Classical-trajectory calculations revealed that fluorocarbon molecules have a non-negligible probability to undergo collision-induced dissociation upon impact with Ar atoms at energies smaller than those available in low-Earth orbit (LEO, 200-700 km altitude). The importance of these results is that non-reactive closed-shell species of the natural LEO atmosphere can degrade polymeric coatings on spacecraft by transferring more energy than is required to break a bond in the surface. Traditionally, the degradation of organic material on the surface of spacecraft operating in LEO has been primarily attributed to hyperthermal (5 eV) atomic oxygen. Even though ground-state atoms of oxygen dominate LEO's atmosphere, there are other gaseous species that might contribute to polymer degradation in spacecraft surfaces. For instance, Ar and N_2 collide with spacecraft surfaces in the RAM direction at energies of 7-12 eV. Even though Ar and N_2 are closed-shell species that cannot degrade organic material through chemical pathways, the collision energy is so large that energy transfer above the dissociation limit of the C-C bonds in the polymer induces degradation via a physical pathway (collision-induced dissociation).

These studies of Ar+C_2H_6 and C_2F_6 hyperthermal collisions required us to carry out expensive high-accuracy ab initio calculations of the intermolecular (Ar-molecule) and intramolecular (C_2H_6 and C_2F_6) potentials. Using ab initio calculations of the Ar-molecule pairs, we derived analytical intermolecular potentials that are general for Ar-alkane and -fluoroalkane hyperthermal interactions. Regarding the C_2H_6 and C_2F_6 intramolecular potentials, we employed the ab initio information to obtain computationally-inexpensive specific-reaction-parameters semiempirical Hamiltonians that possess accuracy comparable to first-principle methods. The SRP Hamiltonians describe appropriately the dissociation energy curves of both the C-X (X=H,F) and C-C bonds in the C_2H_6 and C_2F_6 molecules. The SRP Hamiltonian development in this work drew inspiration from our efforts on direct-dynamics studies of gas-phase reactions mentioned before.

Classical-trajectory calculations using the potentials just described revealed several important results. First, energy transfer to C_2F_6 in hyperthermal Ar collisions is notably more significant than to C_2H_6. This result was ascribed to the presence of more low-frequency vibration modes in the fluorinate molecule, which are efficient energy absorbers. Second, energy transfer above the dissociation limit of the C-X (X=H,F) or C-C bonds of C_2H_6 and C_2F_6 is possible in collisions occurring at energies accessible in LEO environment (up to 12 eV for Ar atoms). In fact, prompt collision-induced dissociation is observed above ~7 eV collision energies. Collision-induced dissociation is more important in fluoroalkanes than in alkanes, and C-C bond breakage is favored over C-X (X=H,F) in both Ar+C_2H_6 and C_2F_6 systems. The results of our chemical-dynamics simulations have been used to inform recent molecular-beam experiments by the Minton group, where degradation of a fluorinated surface upon collision with hyperthermal Ar was observed.

4) Peer-reviewed publications emerging from AFOSR support

1) Hyperthermal Ar atom scattering from a C(0001) surface
K. D. Gibson, S. J. Sibener, Hari P. Upadhyaya, Amy L. Brunsvold, Jianming Zhang, Timothy K. Minton, and Diego Troya
J. Chem. Phys. 128, 224708 (2008)

2) Experimental and theoretical study of CO collisions with CH3- and CF3-terminated self-assembled monolayers
William A. Alexander, John R. Morris, and Diego Troya
J. Chem. Phys. 130, 084702 (2009)

3) Theoretical study of the dynamics of the H+CH4 and H+C2H6 reactions using a specific-reaction-parameter semiempirical Hamiltonian
Joshua P. Layfield, Matthew D. Owens, and Diego Troya
J. Chem. Phys. 128, 194302 (2008)

4) Experimental and theoretical studies of the effect of mass on the dynamics of gas/organic-surface energy transfer
William A. Alexander, B. Scott Day, H. Justin Moore, T. Randall Lee, John R. Morris, and Diego Troya
J. Chem. Phys. 128, 014713 (2008)

5) Barriers of Hydrogen Abstraction from Primary, Secondary, and Tertiary Alkane Sites by O(3P)
Diego Troya
J. Phys. Chem. A 111, 10745 (2007)

6) Theoretical Study of the Ar–, Kr–, and Xe–CH4, –CF4 Intermolecular Potential-Energy Surfaces
William A. Alexander and Diego Troya
J. Phys. Chem. A 110, 10834 (2006)

7) Theoretical Study of the Dynamics of Ar Collisions with C2H6 and C2F6 at Hyperthermal Energy
Uroš Tasić, Pyae Hein, and Diego Troya
J. Phys. Chem. A 111, 3618 (2007)

8) Classical Trajectory Study of the Dynamics of the Reaction of Cl Atoms with Ethane†
Stuart J. Greaves and Andrew J. Orr-Ewing, and Diego Troya
J. Phys. Chem. A 112 9387 (2008)

9) Theoretical Study of the Stereodynamics of CO Collisions with CH3- and CF3-Terminated Alkanethiolate Self-Assembled Monolayers
William A. Alexander, John R. Morris and Diego Troya
J. Phys. Chem. A, Articles ASAP (As Soon As Publishable)

10) Collisions of Polar and Nonpolar Gases with Hydrogen Bonding and Hydrocarbon Self-Assembled Monolayers
Megan E. Bennett, William A. Alexander, Jessica W. Lu, Diego Troya and John R. Morris
J. Phys. Chem. C 112, 17272 (2008)

11) Theoretical study of the dynamics of H+alkane reactions.
Joshua P. Layfield an Diego Troya
Chemical Physics Letters 467, 243 (2009)

12) Theoretical study of the dynamics of hyperthermal collisions of Ar with a fluorinated alkanethiolate self-assembled monolayer.
Uroš Tasić and Diego Troya
Physical Chemistry Chemical Physics 10, 5776 (2008)

13) Direct-dynamics study of the F+CH4, C2H6, C3H8, and i-C4H10 reactions.
Joshua P. Layfield, Andrew F. Sweeney, and Diego Troya
J. Phys. Chem. A, In press