Viewpoints on the 2019 Dynamics of Molecular Collisions Conference

Cite This: J. Phys. Chem. A 2020, 124, 772−780

INTRODUCTION

The inaugural Dynamics of Molecular Collisions (DMC) conference was organized in 1965 by eventual Nobel Prize in Chemistry winner John Fenn (Yale University). The conference has blossomed into a Gordon Research Conference style meeting independently organized by researchers united by the common interest to map the fundamental series of motions that control complex chemical phenomena. DMC conferences are organized every two years with the conference chair alternating between an experimentalist and theoretician to signify the necessity of collaboration. Outstanding theoretical and experimental contributions to the field are recognized at the DMC conference by awarding the Herschbach Medal, a medal named in honor of Dudley Herschbach, Nobel Prize in Chemistry winner in 1986 and a pioneer of the field. In general, the conference includes poster presentations, invited talks, contributed talks, hot topic poster preview talks, and a keynote address organized into different sessions according to the research area. Presentations aim to provide updates on research that address questions in astrochemistry, atmospheric chemistry, and combustion chemistry by studying unimolecular dissociation, bimolecular collisions, cold collisions, quantum control, and interfacial dynamics.

The 27th DMC conference was organized by Timothy Minton (Chair, Montana State University) and Richard Dawes (Co-Chair, Missouri University of Science and Technology) and was held at the Big Sky Resort in Big Sky, Montana, USA, from July 7−12, 2019. Financial support was provided by Montana State University, Johns Hopkins University, and CCS Chemistry/Chinese Chemical Society. Located high in the mountains, countless outdoor activities were available to explore the natural wonders and wildlife of the region. The DMC 2019 conference attendees were presented with a great opportunity to read interviews of Herschbach by John Rigden and Bretislav Friedrich at the end of the conference program. A total of 105 participants were in attendance with more than 65 posters distributed across four evening poster sessions and 43 speakers distributed across 11 presentation sessions. This Viewpoint contains accounts of participating speakers and is grouped according to session title.

HOT TOPICS

Ian Sims (Université de Rennes 1) described the successful use of the CRESU (reaction kinetics in uniform supersonic flow) technique for the determination of gas phase kinetics at temperatures relevant to the astrochemical environment. He highlighted the importance of product branching determination at lower temperatures for astrochemical modeling and described the drawbacks associated with branching ratio determination using the CRESU technique coupled with laser photochemical methods. The CRESU technique coupled with chirped pulse rotational spectroscopy known as chirped pulse in a uniform flow (CPUF) is a time-resolved multiplex detection method that can overcome these issues. Sims and colleagues have developed a new CPUF machine operating in the E band (60−90 GHz) with improved sensitivity. The latest test results from the Rennes CPUF were described, including the detection of the HCN product from the reaction CN + C2H6.

Duncan Bossion (Scribano group, Université de Montpellier) presented an approach to compute thermal rate coefficients at low and high temperatures for astrochemically relevant systems. They have applied the ring polymer molecular dynamics (RPMD) method to study insertion reactions at temperatures ranging from 20−100 K and compared their results with quasiclassical trajectory (QCT) calculations. They have studied the D+ + H2 system, which serves as a prototype for simple ion−molecule reactions [Phys. Chem. Chem. Phys. 2018, 20, 26752−26763 DOI: 10.1039/C8CP05398G]. This reaction does not have an entrance barrier and proceeds through the formation of a long-lived intermediate complex and can exhibit a recrossing effect. Their RPMD calculations intrinsically include this recrossing effect as well as tunneling and show the importance of recognizing this factor in the evaluation of the rate constant. A second calculation was done on a wide temperature range (20−600 K) for the H + HeH+ reaction, which presents a shallow well in the reaction path. The RPMD method showed good agreement with previous quantum calculations and is able to produce thermalized rate coefficients for a wide temperature range using a single method for both insertion and abstraction reactions.

Chandika Amarasinghe (Suits group, University of Missouri-Columbia) studied collisions of highly vibrationally excited molecules at broadly tunable energies by employing a novel home-built dual piezo stack valve where they were able
to create two near-copropagating molecular beams with a 4° intersection angle at the interaction region to reach low collision energies [J. Phys. Chem. Lett. 2019, 10, 2422–2427. DOI: 10.1021/acs.jpcllett.9b00847]. The near copropagating beams allowed them to access collision energies in a broad range from well above room temperature to near 1 K for NO (v = 10)–Ar collisions. In order to accomplish this, they have coupled two powerful techniques, velocity map imaging and stimulated emission pumping (SEP) for the very first time. The SEP method has been employed to prepare NO in a single rovibrational level at v = 10. State-to-state differential cross sections for rotationally inelastic scattering between the state prepared NO and Ar at broad range of collision energies were presented and the results were compared to 2D quantum scattering calculations.

Laura McCaslin (Gerber group, University of California Irvine) discussed recent experimental and theoretical work done to investigate the double photodetachment of the cluster F•H2O in an intense laser field to form [F•H2O]+. This study detected the double photodetachment products H2O+, OH+, O+, HF+, and H2F+. Intrinsic reaction coordinate analysis and ab initio molecular dynamics (AIMD) simulations were performed to characterize the reaction pathway on the lowest-lying triplet and singlet states. The double ionization EOM-CCSD method was chosen for their theoretical study due to the diradical character of the [F•H2O]+ cluster [J. Phys. Chem. Lett. 2018, 9, 6808–6813. DOI: 10.1021/acs.jpcllett.8b02562]. Initial studies were focused on the ground state dynamics and show that the predominant ground state process is separation of H2O+ and F. Moreover, the initial studies also have indicated that formation of OH+, O+, HF+, and H2F+ largely involves excited states and in the case of formation of H2F+, requires excited states. Early AIMD studies of the excited state dynamics of [F•H2O]+ were also presented, unraveling new mechanisms for the formation of H–F bonds.

Uxia Rivero (Willitsch group, University of Basel) presented reactive atomistic simulations of diels-alder reactions involving maleic anhydride and 2,3-dibromo-1,3-butadiene [J. Chem. Phys. 2019, 151, 104301. DOI: 10.1063/1.5114981]. Density functional theory showed that the reaction is symmetric and concerted. Isomerization and fragmentation of the reaction product was found to result in formation of the reactants as most probable dissociation products. In addition, the cross section for the formation of van der Waals complexes diminishes with increasing kinetic energy. The minimum dynamic path indicated that rotational energy is necessary to move the system toward its transition state and that reactive events are rare, needing high rotational energy to proceed.

Fangfang Li (Fengyan Wang group, Fudan University) has studied the oxidation dynamics of metal atoms in the gas phase through crossed molecular beam and time-sliced velocity map imaging. Aluminum or yttrium atoms were collided with O2 at 1.5 and 19.2 kcal/mol, respectively, to form a metal oxide and O(3P). Aluminum oxide was formed via a harpooning mechanism to high rotational levels due to its small rotational constant [Chem. Sci. 2018, 9, 488–494. DOI: 10.1039/C7SC03314A]. Imaging results show that when the collisional orbital angular momentum was nearly completely channeled into the product rotational angular momentum, the maximum of impact parameter was obtained to support the harpooning equation. Velocity and angular distributions of yttrium oxide were also presented, and the complex-formed mechanism was proposed in the oxidation dynamics of the metal atoms.

BIMOLECULAR COLLISION DYNAMICS (CHAIR ED BY AMY MULLIN AND GREG HALL)

Bimolecular collision dynamics have been central to understanding the most detailed information about chemical reactions. DMC 2019 was accompanied by several great presentations spanning from inelastic scattering to reactive scattering studies at both high and low collision energies, and probing geometric phase effects, scattering resonances, vector correlations, nonadiabatic transitions, and construction of novel theoretical methods.

Piergiorgio Casavecchia (University of Perugia) studied the reaction dynamics of O(3P) with unsaturated hydrocarbons utilizing a crossed beam apparatus with universal mass spectrometric detection combined with time-of-flight analysis [J. Phys. Chem. A 2019, 123, 9934–9956. DOI: 10.1021/acs.jpca.9b07621]. The products were probed by using the soft electron ionization method. He emphasized the role of intersystem crossing (ISC) in branching fractions and primary products for these reactions and demonstrated that the intersystem crossing from triplet to the singlet surface increases with increasing lifetime of the triplet intermediate. The experimental results were corroborated by synergistic theoretical calculations of triplet/singlet potential energy surfaces and statistical (RRKM/master equation) computations of branching fractions including ISC.

Astrid Bergeat (Université de Bordeaux) presented experimental results of inelastic collisions between C atoms with He, H2, and D2 utilizing their crossed beam apparatus with variable crossing angle. This apparatus can reduce the intersection angle down to 12.5° and can reach collision energies down to few kelvins where resonance phenomena dominates the collisions. By utilizing a dielectric barrier discharge she was able to prepare C atoms that are mainly in their ground state C(3P0). The state-to-state integral cross sections for spin–orbit excitation of C(3P0) for collisions with He, H2 and D2 were measured using REMPI time-of-flight mass spectrometry [Nat. Chem. 2018, 10, 519–522. DOI: 10.1038/s41557-018-0030-y; J. Phys. Chem. Lett. 2018, 9, 6496–6501. DOI: 10.1021/acs.jpcllett.8b03025; Front. Chem. 2019, 7, 164. DOI: 10.3389/chem.2019.00164]. She further emphasized that these collisions are mainly governed by nonadiabatic processes, and the excellent agreement between experiment results and quantum dynamical calculations validates the accuracy of the calculated potential energy surfaces (PESs). The calculated cross sections can thus be used to model astrophysically related C de/excitation rates in cold molecular clouds.

Bin Zhao (Manthe group, Universität Bielefeld) presented seven-dimensional quantum dynamics calculations studying nonadiabatic transitions in the F(2P) + CHD3 → HF + CD3 reaction. First, global full-dimensional vibrationally and spin–orbit coupled diabatic PESs for this reaction have been discussed. Second, an efficient scheme for performing wave packet propagation on vibronically and spin–orbit coupled surfaces has been described. Finally, reaction dynamics from both the spin–orbit ground and excited electronic states have been presented. This work represents the first quantum scattering calculations to include the nonadiabatic transitions for a system with more than three or four atoms. It reveals that nonadiabatic coupling accounts for 10% of the reactivity of the system.
spin–orbit ground state and that dynamic resonances play an important role. They hope that this work will motivate further studies to probe the vibronic and spin–orbit effects in the entrance channel for many other reactions.

Collisions of ground state NO(X) have been studied extensively by both experimentalists and theorists. However, only a handful of studies have been conducted on its excited state. David Chandler (Sandia National Laboratories) presented a four-vector correlation measurement of molecular scattering by studying the collisions between electronically excited NO(A) with Ne [Nat. Chem. 2018, 10, 1148–1153. DOI: 10.1038/s41557-018-0121-9]. Aligned NO(A) was prepared by circularly polarized light and upon collisions the product alignment was measured. He also discussed the ability of aligning the H2 molecule using electric fields by exploiting the polarizability of H2. By controlling the mixing of E,F and B,C states, he showed the polarizability of H2 can be varied. He concluded that, to date, the mixed E,F state of H2 is the most polarizable state of any molecule. Although Rydberg molecules are polarizable, it is only the electron which will not align the nuclear core.

Marco Panesi’s (University of Illinois at Urbana–Champaign) talk was focused on studying hypersonic aerothermodynamics. He described a reduced order model to accurately calculate the energy transfer and dissociation process in nonequilibrium air mixtures using the coarse-grain quasiclassical trajectory method (CG-QCT). The coarse-grain model combines energy states into groups, and the actual populations is estimated by employing a reconstruction function based on the maximum entropy principle. Afterward, QCT calculations were carried out to compute the group averaged kinetic and thermodynamic group properties. He demonstrated the application of this approach for studying the nonequilibrium relaxation of N2(XΣg−)−N(4Σg) a three-body diatom–atom system, which was found to be in excellent agreement with grouped state-to-state kinetic data [AIP Conference Proceedings 2019, 2132, 140004. DOI: 10.1063/1.5119638]. He also presented their ongoing work on studying the impact of different PESs on the kinetics of O2(XΣg−)−O(3P) [AIAA Aviation 2019 Forum 2019, 3358. DOI: 10.2514/6.2019-3358]. He proposed a novel stochastic approach with the aid of machine learning for carrying out these studies in the future.

Roland Wester (University of Innsbruck) focused his research on obtaining detailed insight into the atomistic dynamics of ion–molecule reactions. Reactions of halogen anions with alkyl halides can proceed along two competing reaction channels, nucleophilic substitution (S2), or base-induced elimination (E2). They have investigated both of these pathways and found that the E2 channel becomes important for ethyl halides employing a crossed molecular beam apparatus with velocity map imaging detection. Different possible reaction mechanisms were revealed by scattering images. Furthermore, they have found that the C–H stretching vibration acts as a spectator mode using vibrationally excited reactants in S2 reactions [Sci. Adv. 2018, 4, eaas9544. DOI: 10.1126/sciadv.aas9544].

Xingan Wang (University of Science and Technology of China) reported their recent and ongoing studies on reactive collisions using a new crossed molecular beam apparatus equipped with a time sliced velocity map imaging detector. By employing near threshold ionization, they have acquired the ion images with very high resolution for the H + HD and F + HD reactions [Science 2018, 362, 1289−1293. DOI: 10.1126/science.aav1356]. These high-resolution results are of great importance in understanding quantum effects in scattering experiments. In particular, the high-resolution results at high collision energy has enabled them to reveal the unique role of geometric phase effect in the H + HD → H2 + D reaction.

### PHOTODISSOCIATION DYNAMICS (CHAIR BY JINGSONG ZHANG)

Photodissociation provides a detailed picture of the molecular dynamics such as cleavage of a bond, internal energy transfers, and radiolysis transitions of a molecule, and it has been used to understand fundamentals of chemical physics ranging from environmental chemistry to attosecond electron dynamics.

Marsha Lester (University of Pennsylvania) discussed the recent studies on the dynamics of the four-carbon Criegee intermediate methyl vinyl ketone oxide derived from isoprene ozonolysis [J. Am. Chem. Soc. 2018, 140, 10866−10880. DOI: 10.1021/jacs.8b06010]. A novel synthetic route has been used to produce Criegee intermediates, and they were characterized by IR action spectroscopy in the C−H stretch overtone region. The unimolecular decay dynamics of Criegee intermediates to OH radical products were detected via UV laser-induced fluorescence, and the energy-dependent OH appearance rates were measured and compared with the theoretical predictions. Moreover, they have observed that the conformation and nature of the substrates of the Criegee intermediate play an important role in reaction dynamics.

Simon North (Texas A&M University) presented findings toward understanding the “odd” behavior in ozone photodissociation [J. Chem. Phys. 2018, 49, 134309. DOI: 10.1063/1.5051540]. In their study, rotational distributions for the O3 fragment were obtained by photodissociation of jet-cooled ozone at three different wavelengths. They have observed the population of rotational distributions alternate between odd and even states, similar to that reported by Valentini et al. However, the alternation is much stronger in the jet-cooled precursors compared to the distributions reported at 300 K and therefore is dependent on parent internal energy. Ion imaging experiments were carried out to study the temperature-dependent vector correlations of the even and odd J states at 266 nm. At all temperatures, the v−j correlations for the j = 19 state were shown to be reduced compared to those of j = 18 and 20, while no such odd/even rotational state difference was observed for the spatial anisotropy, consistent with previous measurements. A simple classical model to treat the effect of parent rotation on the v−j correlation and the odd/even rotational population alternation reproduces both the current measurements and previously reported rotational distributions, suggesting that the “odd” behavior originates from a Λ-doublet propensity, and not from a mass-independent curve crossing effect, as previously proposed.

Benjamin Toulson (Lawrence Berkeley National Laboratory) delivered a talk on probing ultrafast C−Br bond fission in the UV photochemistry of bromoform with femtosecond core-to-valence transient absorption spectroscopy [Struct. Dyn. 2019, 6, 054304. DOI: 10.1063/1.5113798]. Transitions from a core orbital of an atom provide a localized atomic scale perspective, reporting changes in the valence electronic structure with ultrafast time resolution. The XUV spectra at the bromine 3d-edge track how the singly occupied molecular orbitals of transient electronic states develop throughout the C−Br bond fission, eventually forming CHBr2 and Br radicals.
The combination of transient inner-shell spectroscopy with \textit{ab initio} calculations provides detailed insight into the continuous change of electronic orbital characters and transient atomic arrangements during the photochemical process. Two time scales (40 ± 20 and 85 ± 10 fs) dominated changes in the transient absorption spectra, reflecting the different characteristic motions of the light C and H atoms and the heavy Br atoms. A previously proposed, a roaming-mediated ultrafast isomerization pathway could not be reproduced. MD simulations, however, predict that transient isomers may form on time scales of hundreds of femtoseconds, albeit with a lower probability than CHBr$_2$–Br scission.

Jochen Mikosch (Max-Born Institute) is applying tools of attosecond science to molecular dynamics. He and his coworkers have investigated the transient structural dynamics of molecules from a few femtoseconds down to subfemtosecond time scales [\textit{J. Chem. Phys.} 2016, 145, 011101. DOI: 10.1063/1.4955212; \textit{J. Phys. Chem. Lett.} 2019, 10, 265–269. DOI: 10.1021/acs.jpclett.8b02878; \textit{Sci. Adv.} 2018, 4, eaap8148. DOI: 10.1126/sciadv.aap8148]. They have used UV pump–XUV probe femtosecond transient absorption spectroscopy to study the photodissociation dynamics of iodomethane (CH$_3$I) and iodobenzene (C$_6$H$_5$I) in the A band. In this study they have observed migration of a valence shell hole, created by a UV pump pulse, to the iodine reporter atom. Absorption lines converging toward the atomic iodine product appeared promptly with UV absorption for CH$_3$I but were delayed by about 50 fs for C$_6$H$_5$I. They have attributed this delay to the migration of the valence shell hole from the phenyl ring to the reporter atom in C$_6$H$_5$I. The prompt appearance in CH$_3$I, however, was attributed to the hole being created in the iodine lone pair orbital, i.e., centered on the reporter atom. The authors have also explored the electronic state-resolved response of CH$_3$I to a driving IR field in a regime where core-valence and core- to-Rydberg states overlap. Furthermore, they have utilized laser-driven electron diffraction (LIED) in intense infrared fields where a single electron is extracted by laser-driven tunnel ionization, accelerated in the strong field and elastically rescattered with the ion core. Importantly, the experiment separated different continuum channels which elucidates fundamentals of the LIED process.

The electron–electron correlation is central to various processes but has not been thoroughly studied in the time domain due to experimental complexity. One such correlation exists in double ionization process that was addressed by Wen Li (Wayne State University) in his talk. After the ejection of the first electron, the remaining electron density evolves with time in the first femtosecond. To probe these effects, subfemtosecond pump–probe detection capability is required. By using the attosecond two-electron angular streaking method coupled with their new camera-based 3D coincidence imaging detection system, they were able to scan the pump–probe delay from tens of attoseconds to more than 1 fs for the double ionization of benzene. Here the pump–probe refers to the two ionization processes and this study represents the first measurement of electron dynamics in the first 500 attoseconds. They observed a decrease in the double ionization decay rate in the first few hundred attoseconds and concluded that the laser-induced electron correlation is significant in strong field double ionization of benzene initiated by a close-to-circular polarized field [\textit{Phys. Rev. Lett.} 2017, 119, 123201. DOI: 10.1103/PhysRevLett.119.123201].

The concept of potential energy surfaces plays a key role in understanding the fundamentals of chemistry such as dissociation dynamics, spectroscopy, and reaction kinetics. Spiridoula Matsika (Temple University) delivered a presentation on exploring excited state potential energy surfaces for photon and electron-driven processes. In the first part of her presentation she described recent application of both photo-initiated and electron-driven processes involving complex potential energy surfaces on DNA damage and prebiotic chemistry [\textit{Phys. Chem. Chem. Phys.} 2018, 20, 12599–12607. DOI: 10.1039/C8CP0148K]. In one study, her group has utilized a modified electronic structure method for resonances to study how electron attachment to methanol dimers can lead to the formation of sugar precursors. Their results demonstrate that both photons and electrons can facilitate these reactions, but electrons may be more efficient. Evidence for intersystem crossing effects in the exit channel for the reaction of O(3P) and alkylamines was described in the second part of her talk [\textit{Nat. Chem.} 2019, 11, 123–128. DOI: 10.1038/s41557-018-0186-5]. Using multireference perturbation theory \textit{ab initio} calculations, they have found that the reaction is initiated by H abstraction from O attack to produce OH and aminalkyl radicals. The reaction proceeds through intersystem crossing to the singlet surface facilitated by vanishing triplet-singlet splitting and strong spin–orbit coupling in the exit channel of the reaction.

Richard Dawes (Missouri University of Science and Technology) has constructed a new code for the automated construction of potential energy surfaces (PESs) [\textit{J. Chem. Inf. Model.} 2019, 59, 262–271. DOI: 10.1021/acs.jcim.8b00784]. The code is known as AUTOSURF, and the first release of it treats the van der Waals systems as composed of two rigid fragments. The fitting algorithms used in the code have many advanced features such as iterative refinement and symmetry recognition. This code completely automates all of the steps and procedures that go into fitting various classes of PESs and interfaces to popular electronic structure codes such as MOLPRO and GAUSSIAN. The results of dynamics calculations utilizing AUTOSURF were presented for a number of applications including inelastic and photodissociation processes in the atmosphere and interstellar medium. Currently, a new version is under development for reactive systems that contain up to five atoms.

George Schatz (Northwestern University) presented a talk on complex potentials for gas phase and gas–surface reaction dynamics. In the first part of his talk he has reviewed the O(3P) + C$_2$ reaction [\textit{J. Phys. Chem. C} 2012, 116, 26577–26585. DOI: 10.1021/jp3066629]. The reactant C$_2$ can be in two states (C$_2$ $^2 \Sigma_u^+$ and C$_2$ $^3 \Pi_u$) which are separated only by 0.1 eV. C$_2$ $^2 \Sigma_u^+$ gives rise to 9 possible surfaces that have conventional dynamics and C$_2$ $^3 \Pi_u$ leads to 54 surfaces. They have described the reaction dynamics using a statistical approximation to reduce these 54 possible surfaces to 3 surfaces of singlet, triplet, and quintet symmetry, which enable them to use a direct dynamics method. Nonzero cross sections were observed for both ground and excited state products with higher probability forming the latter. In the second part of his talk he described the HYPERthermal reaction O$(^3\Pi)$ + CO$_2$ [\textit{J. Phys. Chem. A} 2011, 116, 64–84. DOI: 10.1021/jp208379j]. This reaction has two major pathways; the low-energy barrier
channel leads to exchange of one oxygen for the other and the higher energy barrier pathway leads to \( \text{O}_2 + \text{CO} \). They have provided mechanisms for both pathways along with concerns related to the product spin states that describe when excited states can be produced by adiabatic dynamics.

**COLLISION DYNAMICS IN THE CONDENSED PHASE (CHAIRIED BY RAFI KAISER)**

Solvents play an important role in dictating the collision dynamics of a reaction. The properties of solutions such as the polarity, hydrogen bonding capability, and vibrational excitation can influence the outcome of chemical reactions. **Andrew Orr-Ewing** (University of Bristol) presented his recent study on chemical dynamics of benzophenone in solution focusing on addressing two key questions: to what extent do the gas phase chemical dynamics apply in solution and can we develop a molecular level picture of solvent influence on ultrafast chemical reaction dynamics [J. Phys. Chem. Lett. 2018, 9, 1642–1648. DOI: 10.1021/acs.jpclett.8b00345; J. Am. Chem. Soc. 2019, 141, 15222–15229. DOI: 10.1021/jacs.9b07047]? Employing the transient absorption spectroscopy technique coupled with ultrafast two-dimensional infrared method, they were able to identify the preferred intersystem crossing (ISC) mechanism \( (S_0(n^*) \rightarrow T_1(n^*)) \) that take place following excitation from \( S_0 \) to \( S_1 \) of benzophenone in methanol. They successfully exploited the red-edge excitation effect (REEE) to selectively photoexcite the benzophenone that contains the carbonyl group coordinated or uncoordinated to the solvent and showed that the extent of hydrogen-bonding interaction determines the rate of ISC. He also demonstrated that the rate of an H abstraction reaction of benzophenone in solution can be increased between 1 and 2 orders of magnitude by using the REEE technique.

**Amanda Case** (Augsburg University) presented their work on vibrationally driven bimolecular reactions in solution. Using their knowledge about vibrational control in the gas phase, they were able to measure H abstraction by a Br atom from vibrationally excited methanol or dimethyl sulfoxide solvents [J. Phys. Chem. B 2017, 121, 2486–2494. DOI: 10.1021/acs.jpcb.7b00035]. Br atoms were produced by photolyzing either bromine or bromoform (\( \text{CHBr}_3 \)), and within the first few picoseconds the radical complexed with the solvent. Employing a near-IR laser pulse, they were able to excite the \( \text{Br}^- \) or \( \text{O} = \text{H} \) stretch of the solvent, thereby enabling the H abstraction reaction, which under thermal conditions is endoergic. By monitoring the decay of the Br–solvent complex using broadband electronic transient absorption, they were able to detect a loss in the reactive bromine indicative of H abstraction. Further measurements showed a decrease in the pH of the solution following vibrational excitation, providing evidence for the formation of the HBr product.

**Ryan Steele** (University of Utah) presented his latest findings on searching for vibrational signatures of strong ion/radical interactions with water. He used a six-dimensional exact eigensolver and an analytic many-body potential energy surface to identify the additional spectral features observed in iodide–water spectra. By including the thermal population of tunnelling-split states, quantum nuclear statistics and asymmetric top rotations with vibrationally averaged rotational constants, he was able to successfully reproduce all the high-frequency structures and most of the low-frequency structures observed in the experimental spectra. In a different study he also demonstrated how the hydration of Cl depends on the size of the Cl(\( \text{H}_2\text{O} \))\(_n\) and addressed its implications on the atmosphere, interstellar medium and in the search for renewable energies [J. Phys. Chem. A 2019, 123, 8657–8673. DOI: 10.1021/acs.jpca.9b07235].

**DYNAMICS OF INTERFACIAL COLLISIONS (CHAIRIED BY STEVEN SIBENER)**

Collision dynamics at the gas–liquid and gas–solid interfaces are essential to many aspects of atmospheric, environmental, and astrochemical processes. Interfaces are important in heterogeneous chemistry and can provide reagents with lower barrier pathways toward chemical reactions that might be kinetically unfavorable in the gas phase. Interaction of gas molecules with aerosol droplets is particularly relevant to atmospheric chemistry, and reactions on the surface of ice grains in space have been implemented in astrochemical models. Thus, an understanding of the fundamentals of energy transfer dynamics in molecular collisions with condensed phase surfaces is essential.

**Kenneth McKendrick** (Heriot-Watt University) highlighted the progress of experimentalists and theoreticians in understanding the dynamics of interfacial collisions. His group has investigated the collision-energy dependence of hydroxyl radical uptake by different liquid surfaces. Hydroxyl radicals exhibited decreasing survival probability across PFPE (assumed to be inert), squalane, and squalene surfaces. A new method was introduced to image scattered molecules in the scattering plane perpendicular to the surface using laser-induced fluorescence [J. Chem. Phys. 2019, 151, 054201. DOI: 10.1063/1.5110517]. Scattered OD on both inert and reactive surfaces exhibited very similar, broad scattering-angle distributions regardless of incident angle. Nonthermal angle-dependent speed distributions were observed, indicating an impulsive scattering mechanism. Imaging of different OD rotational states allowed correlations between angular, speed, and internal distributions to be obtained.

**David Nesbitt** (JILA and University of Colorado Boulder) first presented fully quantum state resolved laser-induced fluorescence measurements of NO evaporating from water [J. Chem. Phys. 2019, 150, 044201. DOI: 10.1063/1.5083050]. NO internal state distributions had rotational and spin–orbit temperatures that are significantly lower than the liquid surface. Furthermore, a larger temperature difference was observed as the jet temperature increased. After accounting for simple evaporative cooling of the liquid microjet, they concluded that weakly supersonic expansion of water molecules away from the microjet in a 1D “slit-like” geometry and partial collisional equilibration of the cooled \( \text{H}_2\text{O} \) with NO via gas phase collisions could be as important as (or potentially even more important than) the nonequilibrium dynamics at the liquid–water surface. Results from thermal and hyperthermal DCl scattering from squalane, PFPE, and glycerol surfaces were also presented [J. Phys. Chem. C 2019, 123, 3449–3460. DOI: 10.1021/acs.jpcc.8b07359]. DCl was probed using narrowband IR laser absorption to achieve rotational and transverse Doppler resolution. The trapping desorption channel was in equilibrium with the liquid. For the impulsive scattering component, the collision energy was efficiently transferred to out-of-plane translational motion while inefficiently partitioning into end-over-end rotation. Results were interpreted in terms of a kinematic “lever arm” collision model and extended to more realistic interfaces.
Simply stated, the microroughness of the liquid surface was found to smooth out sharp rotational rainbow features predicted by the kinematics, providing first insights into why the rotational distributions from highly nonequilibrium impulsive scattering events can be strongly hyperthermal and yet nevertheless Boltzmannesque.

Rebecca Thompson (Sibener group, University of Chicago) introduced a detailed investigation of initial sticking probabilities of CH₄ on various D₂O ice films using in situ reflection absorption infrared spectroscopy [J. Phys. Chem. C 2019, 123, 17855–17863. DOI: 10.1021/acs.jpcc.9b03900]. At the energies studied, CH₄ was unable to embed or significantly alter morphology of the ice films. All surface uptake was found to be from adsorption, and sticking probabilities were relatively consistent between crystalline and nonporous films. High energy CH₄ had significantly higher sticking probability to porous amorphous films, despite the incident energy being well above the barrier for all films. The pore structure was concluded to critically influence adsorption, not necessarily diffusing fully into the pores but allowing for multiple collisions.

Geert-Jan Kroes (Leiden University) presented their work toward providing a chemically accurate description of molecules reacting with transition metal surfaces. By combining the specific reaction parameter approach to density functional theory (SRP-DFT) with direct dynamics, experimental observations of CHD₃ on Ni(111) and Pt(111) were successfully reproduced. A method to develop potential energy surfaces to understand energy transfer between metal surface phonons and polyatomic molecules was also presented. A neural network potential was used to describe CHD₃ on Cu(111) at a considerably reduced computational cost [J. Phys. Chem. Lett. 2019, 10, 1763–1768. DOI: 10.1021/acs.jpclett.9b00560]. Statistically accurate reaction probabilities were obtained, for reaction probabilities as low as 10⁻⁶. The reaction probability was found to be influenced by the bobsled effect and surface recoil. Finally, results from new SRP density functionals based on meta-GGA functionals applied to H₂ + Cu(111) indicated their capability of describing the reaction with chemical accuracy [J. Phys. Chem. A 2019, 123, 5395–5406. DOI: 10.1021/acs.jpca.9b02914].

Tim Schäfer (Georg-August University of Göttingen) reported experimental results published earlier this year on mediation of vibrational relaxation of NO and CO with Ag and Au surfaces [Phys. Chem. Chem. Phys. 2019, 21, 1650–1655. DOI: 10.1039/C8CP06041J]. A unifying relation between the probability of vibrational relaxation was obtained on the basis of the work function of the solid and the electron affinity of the molecule. This suggests that surface to molecule electron transfer is governed by electronically nonadiabatic interactions between nuclear motion and electronic degrees of freedom. In addition, their findings on advancing quantum state resolved surface scattering experiments to nonlinear polyatomic molecules, specifically formaldehyde, were presented. Using a REMPI scheme previously published from his group, formaldehyde molecules were detected and exhibited a propensity for a-axis rotation over b- or c-axis rotation, consistent with a rotational rainbow scattering model [Phys. Chem. Chem. Phys. 2017, 19, 19904–19915. DOI: 10.1039/C7CP03922K]. Finally, chirality detection experiments of fenchone using photoelectron circular dichroism after REMPI demonstrate the ability to obtain a complete picture of surface dynamics of chiral systems [J. Chem. Phys. 2019, 147, 013926. DOI: 10.1063/1.4982614].

QUANTUM CONTROL OF REACTION DYNAMICS (CHAIRIED BY BRIANNA HEAZLEWOOD)

The field of ultracold chemistry is important in understanding the fundamentals of chemical interactions, especially quantum effects. In the recent past many studies have come to light in preparing molecules in this regime. Observing reactions of ultracold samples have generally been limited to measuring the loss rate of the reactants. Kang-Kuen Ni (Harvard University) presented their ongoing work on coupling their optical trap with the ion velocity map imaging technique. Merging of these two methods allowed them to follow the reaction from reactants to products with direct observation of the intermediates. They applied this technique to study the bimolecular reaction between two potassium–rubidium K₉b molecules that were prepared in their lowest ro-vibrational quantum state at 500 nK in their optical trap.

Andreas Osterwalder (EPFL) first presented their ongoing work on scattering of a molecular beam on liquid water utilizing two liquid-microjets. He also demonstrated the use of a beam merging apparatus consisting of two bent quadrupoles and a hexapole to study collisions of two polar molecules. The whole device was fabricated using a 3D printer and partially electroplated to achieve the necessary focusing conditions. The main part of his talk focused on their recent and ongoing work on studying the stereodynamics of reactions between Ne* and Ar or N₂ using the merged beam technique [Nat. Chem. 2018, 10, 1190–1195. DOI: 10.1038/s41557-018-0152-2]. They inferred that by controlling the orientation of Ne* prior to collisions, they were able to control the product branching to Penning ionization products and associative ionization products. This effect was not observed for the low collision energy studies, and he concluded that, at low energies, irrespective of the external field, the Ne* reorients to the most stable configuration. He also briefly discussed a new set of experiments they are pursuing that involves coupling their setup with velocity map imaging detection of the Penning electrons.

Marissa Weichman (Ye group, JILA) presented the very first rotationally resolved spectrum of cold buckminsterfullerene (C₆₀) near the 8.5 m vibrational band [Science 2019, 363, 49–54. DOI: 10.1126/science.aav2616]. The implications of rotationally resolved spectra of fullerenes in chemistry ranges from astrochemistry to quantum computing. The measurement was done by utilizing mid-infrared cavity enhanced frequency comb spectroscopy, and the internal energy of C₆₀ was reduced by cryogenic buffer gas cooling to reduce the spectral congestion. Experimentally observed R branch rotational transitions were successfully reproduced by simulations but fine structure observed in the P branch was not captured by the simulations. This was attributed to “icosahedral splitting” of the degeneracy of J states in the P branch due to nonspherical tensor terms in the rovibrational Hamiltonian. She suggested that future studies of C₁₃₃ may have implications in quantum computing as it forms a spherical lattice network of spin 1/2 nuclei.

Balakrishnan Naduvalath (University of Nevada Las Vegas) presented theoretical studies of ultracold molecular interactions, geometric phase (GP) effect on ultracold state-resolved chemistry, and stereodynamic control of cold collisions. Their recent study of O + OH H + O₂ reaction...
below 1 K revealed large GP effects on state-to-state rotationally resolved rates compared to calculations that did not include the GP effect [Atoms 2019, 7, 65. DOI: 10.3390/atoms7030065]. He also discussed full-dimensional quantum mechanical study of the ultracold K\textsubscript{2} + K\textsubscript{2} + K\textsubscript{2} chemical reaction that revealed signatures of chaotic dynamics and validated the use of the universal model for similar reactions for total reaction rates. The statistical distribution of the product rotational levels was ascribed to the chaotic nature of the reaction complex. In the final part of his talk he described the use of stereodynamics to control the product angular distribution for inelastically scattered HD molecules in collisions with D\textsubscript{2} and H\textsubscript{2} molecules near the cold regime and demonstrated the excellent agreement they observed with recent experiments from the Zare group [Phys. Rev. Lett. 2018, 121, 113401. DOI: 10.1103/PhysRevLett.121.113401; Phys. Rev. Lett. 2019, 123, 043401. DOI: 10.1103/PhysRevLett.123.043401].

Gerrit Groenenboom (Radboud University) proposed a new mechanism for the trap loss of ultracold gases based on their new quasiclassical calculations [Phys. Rev. Lett. 2019, 123, 123402. DOI: 10.1103/PhysRevLett.123.123402]. He first demonstrated the construction of a six-dimensional global PES for NaK + NaK obtained by a Gaussian process regression machine learning fit using fewer than 2500\textsuperscript{ab initio} calculations [J. Chem. Phys. 2019, 150, 064106. DOI: 10.1063/1.5082740]. He then suggested that the long-assumed sticking-enhanced three-body loss mechanism cannot account for the trap loss that has been observed in the experiments. They came to this inference on the basis of their recently derived quasiclassical expression for the density of states of an ultracold, n-atom collision complex [Phys. Rev. A 2019, 100, 032708. DOI: 10.1103/PhysRevA.100.032708]. Instead, the electronic excitations of the collision complexes triggered by the trap laser were determined to be the cause for the trap loss. He proposed using longer wavelengths for the trapping laser or use of repulsive box potentials to reduce the trap loss.

### APPLICATIONS OF MOLECULAR COLLISION DYNAMICS (CHAIR BY ROBERT CONTINETTI)

Studies of molecular collision dynamics have been applied over the years to address frontier questions in atmospheric chemistry, astrochemistry, and combustion chemistry etc. This session consisted of exciting talks ranging from ignition chemistry to nanoparticle surface chemistry.

Craig Taatjes (Sandia National Laboratories) discussed the complex chemical systems in autoignition and tropospheric chemistry where the bimolecular reactions can follow multiple pathways leading to different final products. In ignition chemistry, the formation of reactive radicals can accelerate ignition and formation of closed shell products, which tend to inhibit ignition, was further explained. Furthermore, the application of multiplexed mass spectrometry with tunable synchrotron photoionization that enables the detection and quantification of products and intermediates, sometimes with conformational specificity, was discussed. Methods for direct formation of intermediates, like the reactions that produce carbonyl oxide Criegee intermediates, are key to being able to isolate and measure the reaction kinetics. As an example, the three-step mechanism for ozonolysis of Criegee intermediates and its slow formation compared to the rapid dissociation was discussed. He concluded the talk by presenting the reactivity of Criegee intermediates in different solutions and in the gas phase followed by reactions of conjugated carbonyl oxides from isoprene ozonolysis.

Scott Anderson (University of Utah) has developed an experiment to measure high-temperature reaction kinetics for single nanoparticles (NPs) in the range 5–50 nm confined in a three-dimensional quadrupole trap [Rev. Sci. Instrum. 2014, 85, 014104. DOI: 10.1063/1.4861923], with the goal of studying effects of NP heterogeneity on NP surface chemistry and optical properties. In this experiment, individual NPs are trapped and laser heated, detecting them optically via their thermal emission, allowing the mass to be monitored via the frequency for NP secular motion in the trap. Examples of carbon sublimation and oxidation kinetics were presented, determined by tracking changes in the NP mass vs time as the NPs were heated and exposed to reactants. The NP temperature is determined from the emission spectrum, and Anderson discussed the design of the optical system and an intensity calibration method to enable accurate spectral measurements for single NPs over the 600–1600 nm range [Appl. Opt. 2019, 58, 642–649. DOI: 10.1364/AO.58.000642].

Vanessa Murray (Montana State University) discussed molecular beam–surface scattering experiments on the interactions of hyperthermal O atoms (\(E = 500 \text{\text{kJ mol}}^{-1}\)) with vitreous carbon [J. Phys. Chem. C 2015, 119, 14780–14796. DOI: 10.1021/acs.jpcc.5b00924]. She discussed how the scattered flux of the dominant reaction product (CO) increases continually with surface temperature \((T_s)\) up to \(T_s = 1400 \text{K}\) and then decreases as the \(T_s\) was increased further. Over the same temperature range, O atoms that were initially chemisorbed began to exit the surface. Further studies on the scattering dynamics of hyperthermal O atoms with highly oriented pyrolytic graphite revealed that as \(T_s\) was increased, the desorption barrier for CO increased. This result suggests that O atoms must be present on the surface in order for CO to be released into the gas phase. The combined effects of reduced O atom surface coverage and increased desorption barriers limit the reactivity of the surface at extreme temperatures. A new carbon–oxygen ablation model based on molecular beam experiments was also discussed. It has been used to predict the mass loss of a carbon thermal protection system during hypersonic flight through Earth’s atmosphere.

Gilbert Nathanson (University of Wisconsin, Madison) focused on the substantial impact on climate and air quality by the tiny droplets created by sea spray when bubbles burst at the surface of the ocean. Aerosol droplets scatter sunlight back into space and can indirectly alter the global concentrations of gases such as O\textsubscript{3}, OH, and CH\textsubscript{4}. The concentration of these gases is strongly impacted by the nighttime reactive uptake of dinitrogen pentoxide N\textsubscript{2}O\textsubscript{5}. The concentration of N\textsubscript{2}O\textsubscript{5} varies across different regions because of different organic coatings on the droplet surface. He described the gas–liquid scattering experiments that enabled the development of a “blow-by-blow” description of N\textsubscript{2}O\textsubscript{5}-aerosol reactions. One such instance is the oxidation of dissolved Br\textsuperscript{−} to Br\textsubscript{2} by N\textsubscript{2}O\textsubscript{5} in salty and surfactant-coated water and glycerol. Their microjet and coated-wheel scattering experiments have shown how organic monolayers with different functional groups can catalyze reactions of N\textsubscript{2}O\textsubscript{5} as well as suppress them. He also presented extensive new results on physical properties of N\textsubscript{2}O\textsubscript{5} in or at the surface of water calculated by R. B. Gerber and A. Goetz and co-workers. The main results are obtained using \textit{ab initio} molecular dynamics and calculations of a potential of mean
force. This includes collisions of N₂O₅ with water at 300 K, which lead to extensive trapping at the surface despite a reaction probability of just a few percent [Phys. Chem. Chem. Phys. 2018, 20, 17961–17976. DOI: 10.1039/C8CP03022G].

**KEYNOTE ADDRESS**

The 27th DMC conference invited William L. Hase to deliver the keynote address. Hase is the Robert A. Welch Professor of Chemistry and a Paul Whitfield Horn Professor at Texas Tech University. He is known for his pioneering work in theoretical and computational chemistry, with an emphasis on chemical dynamics. His research started at New Mexico State University where he obtained his Ph.D. He acquired much of his knowledge regarding chemical dynamics simulations as a postdoctoral research associate with Don Bunker at the University of California, Irvine. Awards he has received include Outstanding Performance Award, National Science Foundation, 1985; Lifetime Membership in the Academy of Scholars of Wayne State University, 1994; Distinguished Professor of Chemistry, Wayne State University, 1997–2003; 60th Birthday Special Issue of the International Journal of Mass Spectrometry, Volume 241, Nos. 2–3, 2005; 60th Birthday Festschrift of The Journal of Physical Chemistry A, Volume 110, No. 4, 2006; and Lubbock Chapter, ARCS Foundation, Inc., Scientist of the Year, 2008. He is a Fellow of the American Association for the Advancement of Science and the American Physical Society.

Hase began his talk with a review of the importance, and accuracy and limitations, of chemical dynamics simulations, including a brief description of their methodologies. Direct dynamics, in which the technologies of chemical dynamics and electronic structure theory are coupled, are particularly important and have greatly expanded the range of problems that may be addressed by simulations. For these simulations, parameters required for the dynamics such as potential energy, gradient, and Hessian are obtained directly from electronic structure theory, or by interpolation of the theory, at each numerical integration step of a trajectory. Direct dynamics gives an atomistic understanding of chemical processes and obtains the correct classical dynamics predicted by the electron structure theory. Hase discussed two research areas of his chemical dynamics simulations, e.g., gas–surface energy transfer and gas phase S₂2 reaction dynamics [Phys. Chem. Chem. Phys. 2006, 8, 4678–4684L. DOI: 10.1039/B609743J], Science 2016, 352, 32. DOI: 10.1126/science.aaf5172]. His gas–surface chemical dynamics simulations use analytic potential energy functions for the surface and gas–surface interaction and include collaborations with the experimentalists Julia Laskin, Tim Minton, John Morris, David Nesbitt, Steve Sibener, and many others. He highlighted his simulations of rare gas atoms and CO₂ colliding with self-assembled monolayer surfaces and of O₂ colliding with graphite. Excellent agreement is obtained between simulation and experimental energy transfer dynamics. Hase then talked about the complex nature of gas phase S₂2 reactions and his direct dynamics simulations of these reactions. According to the traditional statistical model, S₂2 reactions proceed via a double well mechanism, with trapping in the wells and RRKM dynamics. However, the actual dynamics is much more complex with multiple mechanisms and nonstatistical dynamics. There are direct mechanisms, such as stripping, and indirect mechanisms such as the roundabout. Microsolvation adds additional complexities to the reaction dynamics. For the OH⁻(H₂O) + CH₃I reaction, there are 28 different indirect atomistic mechanisms! The simulation results are in excellent agreement with experiments by Roland Wester and Al Viggiano.

**HERSCHBACH MEDAL SESSION**

The XXI edition of the DMC meeting in 2007 saw the inaugural pair of awards meant to commemorate outstanding efforts in the field by a pair of researchers, one theoretician, and one experimentalist. The award was christened in the name of Dudley R. Herschbach who received the 1986 Nobel Prize in Chemistry along with Yuan T. Lee and John C. Polanyi for “their contributions concerning the dynamics of chemical elementary processes.” As in past award ceremonies, Herschbach joined the session via Skype and requested the song “Experiment” by Cole Porter be played and embraced by the conference attendees as a virtue by which to live. Herschbach explained the design of the medal, one side which symbolizes the yearning to attain comprehension through theory, the other side symbolizing our grasping for what happens in encounters of atoms, molecules, and/or photons through experiments. The medal also has an unusual, specific shape left for recipients to determine its meaning. Both sides are shown on the cover of the special issue commemorating Fifty Years of Chemical Reaction Dynamics ([J. Phys. Chem. A 2015, 119, 11949. DOI: 10.1021/acs.jpca.5b08530], organized by Hua Guo and Arthur Suits).

After describing the symbolism of the award, Herschbach honored David Yarkony and Kopin Liu for their theoretical and experimental efforts, respectively. Hua Guo introduced David Yarkony and David Chandler introduced Kopin Liu by providing historical pictures from past DMC meetings and providing broad overviews of their seminal contributions to the field.

David Yarkony is the Department of Chemistry Chair and D. Mead Johnson Professor of Chemistry at Johns Hopkins University. His award presentation highlighted his theoretical contributions and was aptly titled “Conical Intersections: After 30 Years Still Surprises”. Prior to his publication in 1990 where he showed that two states of the same symmetry could be connected by conical intersections, they were thought of as only an arcane theoretical notion. Understanding of the dynamics of radiationless decay processes were profoundly altered, and conical intersections were now ubiquitous and viewed as efficient funnels between states. Yarkony presented many molecular systems including vibrationally mediated photodissociation of NH₃ that he called his first success [J. Chem. Phys. 2004, 121, 628. DOI: 10.1063/1.1772351] and fitting conical intersection seams in CH₃NH₂. He also presented results that shifted the paradigm of phenol nonadiabatic dynamics, an impressive feat that he termed the second success given the 33 internal degrees of freedom [J. Chem. Phys. 2014, 140, 024112. DOI: 10.1063/1.4857335]. His research also revealed that the geometric phase effect occurs if there is an accessible path that surrounds the conical intersection regardless of whether the conical intersection itself is energetically accessible. Ground state tunneling in the presence of energetically inaccessible conical intersections and geometric phase limits on single state dynamics were also discussed [J. Am. Chem. Soc. 2018, 140, 1986–1989. DOI: 10.1021/jacs.7b11489].

Kopin Liu is a Distinguished Research Fellow at the Institute of Atomic and Molecular Sciences of Academia Sinica and a Distinguished Research Chair Professor in the
Department of Physics of National Taiwan University. He covered the history of the benchmark F + H$_2$ reaction that helped bring theory and experiment comparisons to the near quantitative agreement that we appreciate today. His work on this system and most notably F + HD identified experimental signatures of quantum dynamical resonances in integral and differential cross sections at a range of collision energies [Phys. Rev. Lett. 2000, 85, 1206–1209. DOI: 10.1021/jacs.7b11489].

Liu spoke on how these experiments laid the foundation for future searches of resonance phenomena and assisted in improvements of potential energy surfaces. After studying A + BC reactions, Liu shifted the paradigm of reaction dynamics by benchmarking the methane + X (X = F, Cl, O(3P), OH) reactions [Chin. J. Chem. Phys. 2019, 32, 1–10. DOI: 10.1063/1674-0068/cjcp1811259]. The varying energetics and barrier heights allowed investigation of how these properties affected reactivity. Product pair correlations, mode and bond selectivity, and steric effects were all advanced as a result of these experiments. In addition, his contributions to the development of velocity map imaging for crossed molecular beam experiments cannot be understated. He concluded his presentation by presenting new results on acetaldehyde photodissociation at different energies than previously studied. By imaging CO, new roaming dynamics to produce CH$_4$ were revealed distinct from photodissociation of formaldehyde.

**CONCLUSION**

The DMC conference continues to serve as a venue to unite the brightest minds in physical chemistry and stimulate discussions on the frontiers of chemical dynamics. Organizing a conference is a huge burden to bear and was brilliantly accomplished due to the heroic efforts of the conference site staff and conference organizers Timothy Minton and Richard Dawes. The generous financial support from Montana State University, Johns Hopkins University, and CCS Chemistry/Chinese Chemical Society was greatly appreciated. We thank the speakers for presenting important recent progress from their groups and appreciate the session chairs for guiding the discussions. The keynote address by Bill Hase on the comparison of experiment and theoretical models emphasized the spirit of the meeting, and the introduction of Kopin Liu and David Yarkony by Dudley Herschbach showed the great progress of the field throughout their careers. We thank all poster presenters and acknowledge the poster prize winners Chandika Amarasinghe (Suits group, University of Missouri), Michael Vansco (Lester group, University of Pennsylvania), and Marissa Weichman (Ye group, JILA). The 28th DMC will continue the tradition of excellence in 2021 with Richard Dawes and Amy Mullin as Chair and Co-Chair from July 11th to 16th at Snowbird, Utah.

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Notes

The authors declare no competing financial interest.