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14. ABSTRACT

15. SUBJECT TERMS

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Svetlana Kotochigova
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RPPR Final Report
as of 15-Oct-2021

Agency Code: 21XD

Proposal Number: 69178CH **Agreement Number: W911NF-17-1-0563**

INVESTIGATOR(S):

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Principal: Y

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DUNS Number: 057123192 EIN: 231365971
Report Date: 14-Jul-2021 Date Received: 12-Jun-2021
Final Report for Period Beginning 15-Sep-2017 and Ending 14-Apr-2021
Title: Effect of conical intersections on chemical reactivity of ultracold molecules in optical potentials
Begin Performance Period: 15-Sep-2017 **End Performance Period:** 14-Apr-2021
Report Term: 0-Other
Submitted By: Svetlana Kotochigova Email: skotoch@temple.edu
Phone: (215) 204-3777
Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: **STEM Participants:**

Major Goals: Conical intersections between molecular electronic potential surfaces can greatly affect molecular dynamics and chemical properties. The different conditions under which and the effect of these conical intersections occur have been extensively described in the literature. These studies, however, were mostly restricted to temperatures above 1 K, where typically many angular momenta or partial waves contribute to the overall reaction outcome. Remarkable progress in cooling and trapping molecules in recent years has opened up an entirely new energy regime: chemical reactivity at temperatures below one milli-Kelvin and even one micro-Kelvin. Then quantum interference effects and threshold phenomena begin to dominate in collisions as only few partial waves contribute and multiple reaction pathways interfere. In addition, it is possible to prepare these molecules in unique rovibrational states and turn on and off the effect of conical intersections. These novel capabilities pave the way to explore the fundamental principles of molecular reactivity at the very quantum limit. The objectives of the reported research were to develop theoretical models of and practical applications for conical intersections with their geometric phases to ultracold chemical reactions with molecules confined and controlled in optical potentials. The primary research focus was aimed at describing the collision among heteronuclear polar molecules, cooled to ?K temperatures, as well as the collision of these molecules with ultracold atoms. In addition, we studied means to control the charge-exchange reaction of atoms and ions with laser light and how to form and trap the heteronuclear polar molecules. In this report, we summarize our accomplishments under Grant W911NF-17-1-0563. For these efforts, five topics always needed to be addressed or considered: 1) Carry out detailed electronic structure calculations of polyatomic complexes; 2) Locate and determine properties of conical intersections for the different molecular systems; 3) Developed numerical quantum mechanical methods and perform quantum dynamics calculations of state-to-state reaction rate coefficients that include the quantum interference due to conical intersections. 4) Search for the dynamic signatures of passage around conical intersections to distinguish between relaxation and reaction pathways; and 5) For reactive systems analyze the effect of conical intersections on the distribution of vibrationally and rotationally resolved rates in product molecules. Detailed information regarding our accomplishments is given below.

The principal investigator (PI) for these efforts is Professor Svetlana Kotochigova. She was assisted by graduate and postgraduate research assistants. The reported research has a broad interdisciplinary impact as both physicists and chemists worked to explore new classes of molecular species and develop new methods to study their chemical reactivity. The results of this study helped to set up realistic models for experiments on chemical reactions at Harvard University, CalTech, and Duke University in the USA, and a Max-Planck Institute in Germany. These collaborations led to a validation of the collisional properties for selected molecules and to improved quantum-state preparation of these molecules. The PI also provided much needed scientific information to leading theoretical groups at two National Laboratories, LANL and NIST, as well as the University of Nevada and Harvard University. This information included electronic potential energies, analyses of derivative couplings between PESs, and setting up a rigorous study of the properties of conical intersections. The ARO supported research resulted in twenty peer-reviewed published papers.

Accomplishments: See attached pdf file

Training Opportunities: PI will set up a training program for the graduate students and postdoctoral researchers. This program includes:
- PI established regular twice-weekly meetings to discuss research progress;
- The postdoc researchers helped supervise the graduate students;
- Training to work on state-of-the art computational programs that help to underpin calculation of electronic structure and trapping condition for dimers and polyatomic molecules;
- PI gave guidance on how collaborate with theoretical and experimental researches;
- Training to write research papers;
- Prepare and give presentations at conferences.

Participating in the ARO supported research researchers explored the new and exciting field of quantum information and quantum chemistry as well as research at the frontier of computational physics.

Results Dissemination: See attached pdf file for a list of 20 peer-reviewed publications supported by ARO Grant. In addition, the pdf file contains a list of invited talks by the PI at National and International meetings and conferences.

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI
Participant: Svetlana Kotochigova
Person Months Worked: 8.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Ming Li
Person Months Worked: 12.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Graduate Student (research assistant)
Participant: Constantinos Makrides
Person Months Worked: 6.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Staff Scientist (doctoral level)
Participant: Jacek Klos
Person Months Worked: 5.00 **Funding Support:**
Project Contribution:
National Academy Member: N

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Participant Type: Graduate Student (research assistant)
Participant: Chi Hong Yuen
Person Months Worked: 3.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Non-Student Research Assistant
Participant: Hui Li
Person Months Worked: 4.00 **Funding Support:**
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Date Submitted: 8/6/18 12:00AM Date Published: 7/1/17 8:00AM
Publication Location: Philadelphia, PA, United States
Article Title: Universality and chaoticity in ultracold K+KRb chemical reactions
Authors: J. F. E. Croft, C. Makrides, M. Li, A. Petrov, B. K. Kendrick, N. Balakrishnan, S. Kotochigova
Keywords: chemical reactivity, reaction dynamics, conical intersections, chaos
Abstract: A fundamental question in the study of chemical reactions is how reactions proceed at a collision energy close to absolute zero. This question is no longer hypothetical: quantum degenerate gases of atoms and molecules can now be created at temperatures lower than a few tens of nanokelvin. Here we consider the benchmark ultracold reaction between, the most-celebrated ultracold molecule, KRb and K. We map out an accurate ab initio ground-state potential energy surface of the K2Rb complex in full dimensionality and report numerically-exact quantum-mechanical reaction dynamics. The distribution of rotationally resolved rates is shown to be Poissonian. An analysis of the hyperspherical adiabatic potential curves explains this statistical character revealing a chaotic distribution for the short-range collision complex that plays a key role in governing the reaction outcome.
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
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Publication Location: Philadelphia, PA, United States
Article Title: Orbital quantum magnetism in spin dynamics of strongly interacting magnetic lanthanide atoms
Authors: Ming Li, Eite Tiesinga, Svetlana Kotochigova
Keywords: quantum magnetism, spin evolution, optical lattice
Abstract: Laser cooled lanthanide atoms are ideal candidates with which to study strong and unconventional quantum magnetism with exotic phases. Here, we use state-of-the-art closed-coupling simulations to model quantum magnetism for pairs of ultracold spin-6 erbium lanthanide atoms placed in a deep optical lattice. In contrast to the widely used single-channel Hubbard model description of atoms and molecules in an optical lattice, we focus on the single-site multi-channel spin evolution due to spin-dependent contact, anisotropic van der Waals, and dipolar forces. This has allowed us to identify the leading mechanism, orbital anisotropy, that governs molecular spin dynamics among erbium atoms. The large magnetic moment and combined orbital angular momentum of the 4f-shell electrons are responsible for these strong anisotropic interactions and unconventional quantum magnetism.
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Publication Location: Philadelphia, PA, United States
Article Title: Fractal universality in near-threshold magnetic lanthanide dimers
Authors: Constantinos Makrides, Ming Li, Eite Tiesinga, Svetlana Kotochigova
Keywords: Quantum Chaos, Disorder, Ergodic Systems, Universality in molecular interactions
Abstract: Ergodic quantum systems are often quite alike, whereas nonergodic, fractal systems are unique and display characteristic properties.We explore one of these fractal systems, weakly bound dysprosiumlanthanide molecules, in an external magnetic field. As recently shown, colliding ultracold magnetic dysprosium atoms display a soft chaotic behavior with a small degree of disorder. We broaden this classification by investigating the generalized inverse participation ratio and fractal dimensions for large sets ofmolecular wave functions. Our exact close-coupling simulations reveal a dynamic phase transition frompartially localized states to totally delocalized states and universality in its distribution by increasing the magnetic field strength to only a hundred Gauss (or 10 mT). Finally, we prove the existence of nonergodic delocalized phase in the system and explain the violation of ergodicity by strong coupling between near-threshold molecular states and the nearby continuum.
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Volume: 121 Issue: First Page #: 253401
Date Submitted: 7/25/19 12:00AM Date Published: 12/19/18 5:00AM
Publication Location:
Article Title: Extending Rotational Coherence of Interacting Polar Molecules in a Spin-Decoupled Magic Trap
Authors: Frauke Seeßelberg, Xin-Yu Luo, Ming Li, Roman Bause, Svetlana Kotochigova, Immanuel Bloch, and
Keywords: polar molecule, coherent control
Abstract: Superpositions of rotational states in polar molecules induce strong, long-range dipolar interactions. Here we extend the rotational coherence by nearly 1 order of magnitude to 8.7(6) ms in a dilute gas of polar 23Na40K molecules in an optical trap. We demonstrate spin-decoupled magic trapping, which cancels first- order and reduces second-order differential light shifts. The latter is achieved with a dc electric field that decouples nuclear spin, rotation, and trapping light field. We observe density-dependent coherence times, which can be explained by dipolar interactions in the bulk gas.
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Date Submitted: 7/25/19 12:00AM Date Published: 3/15/19 4:00AM
Publication Location: Basel, Switzerland
Article Title: Universal Scattering of Ultracold Atoms and Molecules in Optical Potentials
Authors: Hui Li, Ming Li, Constantinos Makrides, Alexander Petrov, and Svetlana Kotochigova
Keywords: ultracold atom-molecule collisions; chemical reactions; universal model; dispersion interaction; van der Waals coefficients; dynamic polorizability
Abstract: Universal collisions describe the reaction of molecules and atoms as dominated by long- range interparticle interactions. Here, we calculate the universal inelastic rate coefficients for a large group of ultracold polar molecules in their lower ro-vibrational states colliding with one of their constituent atoms. The rate coefficients are solely determined by values of the dispersion coefficient and reduced mass of the collisional system. We use the ab initio coupled-cluster linear response method to compute dynamic molecular polarizabilities and obtain the dispersion coefficients for some of the collisional partners and use values from the literature for others. Our polarizability calculations agree well with available experimental measurements. Comparison of our inelastic rate coefficients with results of numerically exact quantum-mechanical calculations leads us to conjecture that collisions with heavier atoms can be expected to be more universal.
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Date Submitted: 7/25/19 12:00AM Date Published: 6/14/19 4:00AM
Publication Location: United States
Article Title: Engineering Excited-State Interactions at Ultracold Temperatures
Authors: Michael Mills, Prateek Puri, Ming Li, Steven J. Schowalter, Alexander Dunning, Christian Schneider, Sve
Keywords: charge transfer reaction, excited state chemistry, non-adiabatic coupling
Abstract: Using a recently developed method for precisely controlling collision energy, we observe a dramatic suppression of inelastic collisions between an atom and ion (Ca + Ybþ) at low collision energy. This suppression, which is expected to be a universal phenomenon, arises when the spontaneous emission lifetime of the excited state is comparable to or shorter than the collision complex lifetime. We develop a technique to remove this suppression and engineer excited-state interactions. By dressing the system with a strong catalyst laser, a significant fraction of the collision complexes can be excited at a specified atom-ion separation. This technique allows excited-state collisions to be studied, even at ultracold temperature, and provides a general method for engineering ultracold excited-state interactions.
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: PHYSICAL REVIEW A
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Volume: 99 Issue: First Page #: 062706
Date Submitted: 7/25/19 12:00AM Date Published: 6/14/19 4:00AM
Publication Location: United States
Article Title: Excitation-assisted nonadiabatic charge-transfer reaction in a mixed atom-ion system
Authors: Ming Li, Michael Mills, Prateek Puri, Alexander Petrov, Eric R. Hudson, and Svetlana Kotochigova
Keywords: charge transfer reaction, excited state chemistry, coupled-channels modeling
Abstract: An important physical process unique to neutral-ion systems is the charge-transfer reaction. Here, we present measurements of and models for charge-transfer processes between cotrapped ultracold Ca atoms and Yb ions under well-controlled conditions. The theoretical analysis suggests the existence of three reaction mechanisms when lasers from a magneto-optical trap and an additional catalyst laser are present. We show that the near-degeneracy of the excited Ca(1P1) + Yb+(2S) and Ca+(2S) + Yb(3D2) asymptotic limits leads to large charge-transfer rate coefficients that can be controlled by changing the frequency of the catalyst laser and the ion temperature. Our model agrees with experimental rate-coefficient measurements between 50 mK and 1 K, with and without the catalyst laser, using just a single free parameter.
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Publication Location: United States
Article Title: Two-photon photoassociation spectroscopy of the 2??\Sigma+ YbLi molecular ground state
Authors: Alaina Green, Jun Hui See Toh, Richard Roy, Ming Li, Svetlana Kotochigova, and Subhadeep Gupta
Keywords: ultracold molecules, photoassociation, scattering length

Abstract: We report on measurements of the binding energies of several weakly bound vibrational states of the paramagnetic 174Yb6Li molecule in the electronic ground state using two-photon spectroscopy in an ultracold atomic mixture confined in an optical dipole trap. We theoretically analyze the experimental spectrum to obtain an accurate description of the long-range potential of the ground-state molecule. Based on the measured binding energies, we arrive at an improved value of the interspecies s-wave scattering length as0 = 30 a0. Employing coherent two-photon spectroscopy we also observe the creation of “dark” atom-molecule superposition states in the heteronuclear Yb-Li system. This paper is an important step towards the efficient production of ultracold YbLi molecules via association from an ultracold atomic mixture.

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors
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Partners

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I certify that the information in the report is complete and accurate:
Signature: Svetlana Kotochigova
Signature Date: 6/12/21 6:36PM

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Dr. Svetlana Kotochigova

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College of Science and Technology
Temple University
Philadelphia, PA 19122

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14. ABSTRACT

This final report summarizes our accomplishments over the 3.5 years of support under this grant. The first thrust focused on the role of non-adiabatic coupling in reactive and non-reactive scattering of ultracold neutral molecules. This involved quantum-mechanical studies of atom-molecule reactions as well as hyperfine quenching of hydroxyl OH in collisions with ultracold Sr atoms. The calculations included conical intersections between potential surfaces. The second thrust concentrated on the investigation of non-adiabatic processes in charge-exchange reactions. The third trust analyzed various factors that affect the photo-associative formation of cold molecules under the influence of external fields. The final trust was related to modeling of dephasing and decoherence processes of ultracold molecules prepared in superposition states and held in place by external trapping light. Our research has resulted in 20 articles in peer-reviewed journals, such as Nature, Science Adv., Phys. Rev. X, and Phys. Rev. Lett. PhandRev.Lett.anPhys.Chem.Chem.Phys. and others. The efforts led to improved theoretical understanding of the role that conical intersections play in reactions with and relaxation in ultracold molecules. In addition, we developed new means to form and control

15. SUBJECT TERMS
Non-adiabatic coupling, conical intersections, ultracold molecules, electronic structure polyatomic molecules, reactive scattering, chemical reactivity, external electric and magnetic fields.

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19a. NAME OF RESPONSIBLE PERSON
Svetlana Kotochigova

19b. TELEPHONE NUMBER *(Include area code)*
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College of Science and Technology
Physics department of
Temple University
Philadelphia, PA

Final Report for
Grant W911NF-17-1-0563

Effect of conical intersections on chemical reactivity of ultracold molecules in optical potentials

Principal Investigator:
Prof. Svetlana Kotochigova
email: skotoch@temple.edu

Submitted to:

Dr. James Parker,
Program Officer, Chemical Science Division
Army Research Office
Research Triangle Park, NC 27709-2211

June 12, 2021

Summary: Objectives and Status of Effort

Conical intersections between molecular electronic potential surfaces can greatly affect molecular dynamics and chemical properties. The different conditions under which and the effect of these conical intersections occur have been extensively described in the literature. These studies, however, were mostly restricted to temperatures above 1 K, where typically many angular momenta or partial waves contribute to the overall reaction outcome. Remarkable progress in cooling and trapping molecules in recent years has opened up an entirely new energy regime: chemical reactivity at temperatures below one milli-Kelvin and even one micro-Kelvin. Then quantum interference effects and threshold phenomena begin to dominate in collisions as only few partial waves contribute and multiple reaction pathways interfere. In addition, it is possible to prepare these molecules in unique rovibrational states and turn on and off the effect of conical intersections. These novel capabilities pave the way to explore the fundamental principles of molecular reactivity at the very quantum limit.

The objectives of the reported research were to develop theoretical models of and practical applications for conical intersections with their geometric phases to ultracold chemical reactions with molecules confined and controlled in optical potentials. The primary research focus was aimed at describing the collision among heteronuclear polar molecules, cooled to μK temperatures, as well as the collision of these molecules with ultracold atoms. In addition, we studied means to control the charge-exchange reaction of atoms and ions with laser light and how to form and trap the heteronuclear polar molecules. In this report, we summarize our accomplishments under Grant W911NF-17-1-0563. For these efforts, five topics always needed to be addressed or considered: 1) Carry out detailed electronic structure calculations of polyatomic complexes; 2) Locate and determine properties of conical intersections for the different molecular systems; 3) Developed numerical quantum mechanical methods and perform quantum dynamics calculations of state-to-state reaction rate coefficients that include the quantum interference due to conical intersections. 4) Search for the dynamic signatures of passage around conical intersections to distinguish between relaxation and reaction pathways; and 5) For reactive systems analyze the effect of conical intersections on the distribution of vibrationally and rotationally resolved rates in product molecules. Detailed information regarding our accomplishments is given below.

The principal investigator (PI) for these efforts is Professor Svetlana Kotochigova. She was assisted by graduate and postgraduate research assistants. The reported research has a broad interdisciplinary impact as both physicists and chemists worked to explore new classes of molecular species and develop new methods to study their chemical reactivity. The results of this study helped to set up realistic models for experiments on chemical reactions at Harvard University, CalTech, and Duke University in the USA, and a Max-Planck Institute in Germany. These collaborations led to a validation of the collisional properties for selected molecules and to improved quantum-state preparation of these molecules. The PI also provided much needed scientific information to leading theoretical groups at two National Laboratories, LANL and NIST, as well as the University of Nevada and Harvard University. This information included electronic potential energies, analyses of derivative couplings between PESs, and setting up a rigorous study of the properties of conical intersections. The ARO supported research resulted in twenty peer-reviewed published papers.

Accomplishments

1 Non-adiabatic coupling in reactive scattering and hyperfine quenching with ultracold molecules

In this section we describe our investigations into chemical reactivity and hyperfine-state changing collisions between small molecules and atoms at temperatures below a few milli-Kelvin. We found strong effects of non-adiabatic passage through conical intersections (CIs) and of the geometric phases (GPs) induced by the CI on relaxation and reaction pathways. Specifically, our simulations demonstrated the existence of quantum interference in ultracold molecular collisions.

1.1 Atom-molecule reaction over the conical intersection

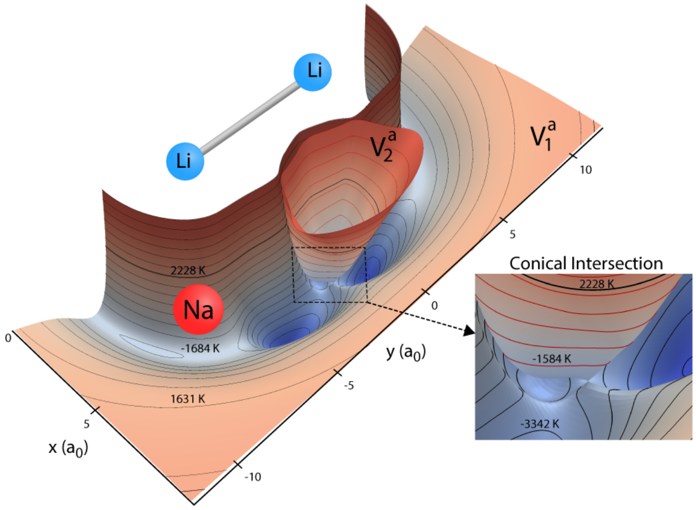

Figure 1: The two energetically-lowest doublet potential energy surfaces, labeled V_1^a and V_2^a, for Li_2Na as functions of the location of the Na atom at a fixed Li_2 bond length of $6.25a_0$, where a_0 is the Bohr radius. The excited-state surface has a conical intersection with the ground-state surface for T-shaped geometries. Contour energies in Kelvin are relative to the minimum energy of the ground electronic state of the Li_2 + Na dissociation limit.

We showed from first principles and for the first time that CI-induced non-adiabatic quantum dynamics is important in reactive scattering between ultracold LiNa alkali-metal molecules and ultracold Li atoms. This dynamics contains quantum interferences that dramatically alter the vibrationally- and rotationally-resolved rate coefficients for products $\mathrm{Li}_2(v', j')$. The rate coefficient summed over product ro-vibrational states, however, is insensitive to the presence of non-adiabatic dynamics. Interference effects tend to wash out in a sum over final states.

The relevant potential energy surfaces (PESs) of trimer Li_2Na were not available from the literature and their computation required substantial effort. We computed the two energetically-lowest doublet *adiabatic* potentials, ${}^2A'$ and ${}^2B'$, using the non-relativistic multi-reference configuration-interaction (MRCI) method with a large active space. We also needed to *diabatize* these two three-dimensional (3D) potentials, in order to isolate the conical intersection at C_{2v} symmetry, *i.e.* equilateral triangle geometries. Figure 1 shows two 2D cross sections through the adiabatic potentials. For an ultracold collision between LiNa and Li *both* ground and first-excited electronic states are energetically accessible in the interaction region where all three atoms are close together. Thus, both potentials and their coupling must be included in quantum dynamics calculations. The non-adiabatic couplings are strongest near the conical intersection. As discussed in detail in our recent publication, the CI leads to dramatic changes in the variations in the ro-

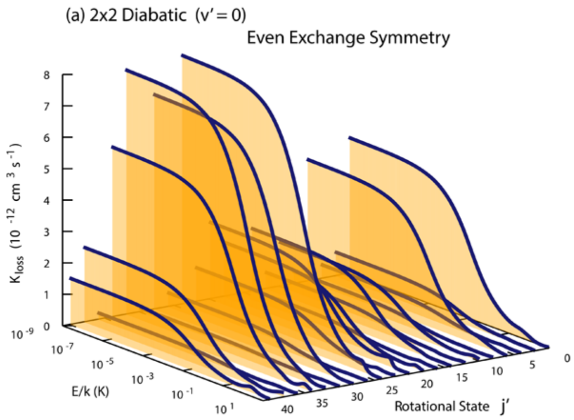

Figure 2: Rotationally-resolved rate coefficients for the Li + LiNa$(v = 0, j = 0) \to \mathrm{Li}_2(v' = 0, j')$ + Na reaction as functions of relative collision energy E and j' with even exchange symmetry. The left and right panels show rate coefficients computed using two coupled diabatic surfaces and with a single adiabatic surface, respectively.

tationally resolved rate coefficients. Figure 2 gives an example of the rotationally resolved rate coefficients for the Li + LiNa$(v = 0, j = 0) \to \mathrm{Li}_2(v' = 0, j')$ + Na reaction as functions of collision energy and product rotational state j'. The j' distribution of rate coefficients changes noticeably when the non-adiabatic coupling is removed.

1.2 Universality and quantum chaos in ultracold reactions between molecules and atoms

Several fundamental questions in the study of chemical reactions at a collision energy close to absolute zero must answered. One is the presence of so-called quantum chaos. For this purpose, we considered the benchmark ultracold reaction between KRb, the most-celebrated ultracold molecule, and K as well as the reaction of LiYb with Li. For the first time, we mapped out accurate *ab initio* ground-state potential energy surfaces of the K_2Rb and Li_2Yb complexes in their full dimensionality and reported on numerically exact quantum-mechanical reaction dynamics. A statistical analysis of the "hyperspherical adiabatic" potentials derived from these *ab initio* PESs shows that the short-range

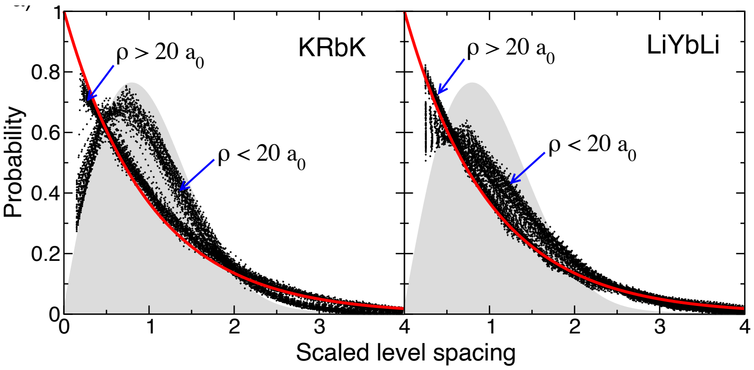

Figure 3: Statistical analysis of the short-range trimer potentials for K_2Rb (left panel) and Li_2Yb (right panel). The graphs show distributions of nearest-neighbor spacings of adiabatic potential energies in hyperspherical coordinates as functions of scaled level spacing. Each black dotted curve corresponds to the distribution for a single hyperradius ρ. The shaded grey area and red curve are Wigner-Dyson and Poisson distributions, respectively. Only curves for total trimer angular momentum $J = 0$ are shown.

trimer complexes have chaotic distributions and play a key role in the reaction outcomes.

Specifically, we analyzed the thousands of adiabatic potentials in the hyperspherical coordinate system for various values of hyperradius ρ, a well-defined measure of the size of the trimers. The appeal of this approach is that it allowed us to compare the short- and long-range interactions in order to understand their effect on the reaction dynamics. We analyzed the distribution of nearest-neighbor level-spacings among these adiabatic potentials using random matrix theory. Figure 3a shows these distributions for K_2Rb and Li_2Yb as functions of spacing between the potentials. Each curve corresponds to a normalized distribution for one hyperradius, where spacings are scaled by the mean spacing at this radius. For K_2Rb, we can identify two general trends in the distributions depending on the value of the hyper radius ρ. For $\rho < 20a_0$, defining the collisional complex, the distribution among the hyperspherical adiabatic potentials are close to the Wigner-Dyson distribution characteristic of quantum chaos, due to strong interactions between the potentials. The situation dramatically changes at larger ρ, where reactant and product states are energetically well separated. Here, the distribution is described by a Poisson distribution corresponding to statistical disorder. A comparison of the distributions for K_2Rb and Li_2Yb shows that the chaotic regime for smaller ρ is more pronounced in K_2Rb than for Li_2Yb. We have attributed this to the much higher density of states of K_2Rb.

1.3 Effects of a CI on the hyperfine quenching of radical OH colliding with ultracold Sr

The role of conical intersections on electronic relaxation, transitions from excited electronic states to ground states, is well studied. Their influence on non-reactive hyperfine quenching is not. We reported on ultracold non-reactive collisions of the free-radical OH with Sr leading to quenching of OH hyperfine states. Our quantum-mechanical calculations of this process revealed that quenching is efficient due to anomalous molecular dynamics in the vicinity of the conical intersection at a collinear geometry. We observed "wide" scattering resonances in both elastic and inelastic rate coefficients at collision energies below $k_B \times 10$ mK, where k_B is the Boltzmann constant. They were identified as either due to *p*- or *d*-wave shape resonances.

As a first step, we computed the *ab-initio* adiabatic SrOH electronic potentials and set up a diabatization procedure near the CIs. Diabatic potential surfaces and their couplings were determined from non-relativistic coupled-cluster electronic-structure calculations with single, double, and perturbative triple excitations and the equation-of-motion coupled-cluster method. Three non-relativistic *diabatic* surfaces are relevant: one is a deep ionically-bound potential, labeled by symmetry $1\,^2A'$, and two are shallow nearly-degenerate van-der-Waals-bonded potentials, labeled by $4\,^2A'$ and $4\,^2A''$, that dissociate to ground-state Sr(^{1}S) and OH(X$^2\Pi$), respectively. The $1\,^2A'$ state dissociates to an electronically excited OH molecule and CIs exists between the two $^2A'$ potentials at linear geometries.

We also had to develop a coupled-channels model to determine atom-dimer quenching rate coefficients for ^{88}Sr+^{16}OH at collision energies below $k_B \times 10$ mK. The model includes the three diabatic non-relativistic trimer potential surfaces and their couplings as well as spin-orbit, rotational, Λ-doubling, and hyperfine interactions in the OH dimer. The OH stretch was modeled by the $v = 0$ vibrational eigenstate of the OH dimer for all $^2A'$ and $^2A''$ symmetries. Many rotational and spin-orbit states were included.

Figure 4 shows our predictions for elastic and inelastic hyperfine-quenching rate coefficients when the $J = 3/2$ OH(X$^2\Pi_{3/2}$) rotational state is prepared in hyperfine-resolved states $|e; F = 2\rangle$

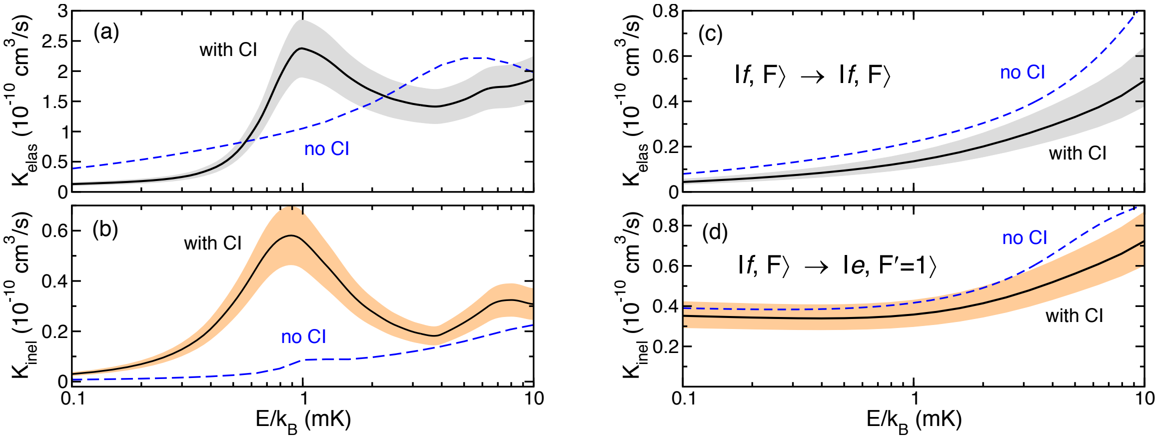

Figure 4: Total elastic [panels (a) and (c)] and inelastic [panels (b) and (d)] rate coefficients as functions of relative collision energy E for the ^{88}Sr and $v = 0, J = 3/2$ ^{16}OH($X^2\Pi_{3/2}$) collision. Solid and dashed curves give calculations with and without the conical intersection between $1\,^2A'$ and $4\,^2A'$ potentials, respectively. Grey and orange bands indicate the uncertainties in rate coefficients due to our inability to include all rotational states of OH when the CI is included in the calculations. Panels (a) and (b) show total elastic and partial inelastic hyperfine quenching rate coefficients for OH in its $|e; F = 2\rangle$ hyperfine state, whereas panels (c) and (d) show rate coefficients for OH in its $|f; F = 1\rangle$ and $|f; F = 2\rangle$ hyperfine states. Rate coefficients for $|f; F = 1\rangle$ and $|f; F = 2\rangle$ are indistinguishable on the scale of the figure.

or $|f; F = 1, 2\rangle$ quenching to state $|e; F' = 1\rangle$. We found that rate coefficients for initial state $|e; F = 2\rangle$ have a strong resonance near $E = k_B \times 1$ mK, but only when the coupling between the $1\,^2A'$ and $4\,^2A'$ states is switched on. For this initial state the elastic rate coefficients were about five time larger than the inelastic ones. Rate coefficients for initial states $|f; F = 1, 2\rangle$ had no resonances and elastic and inelastic rate coefficients are nearly the same.

2 Non-adiabatic atom-ion charge-transfer reactions

A physical process unique to mixed neutral and ion systems is the charge-transfer reaction. We investigated this reaction in the collision between an electronically excited laser-cooled Ca atom with a cold ytterbium Yb$^+$ ion kept in a Penning ion trap. (We also studied a similar process in K + Ca$^+$.) First, we note that ground state Ca(^{1}S$_0$) and ground state Yb$^+$(^{2}S$_{1/2}$) react to create Ca$^+$ and Yb at a currently unobservable small rate. Instead, we suggested the existence of an additional charge-transfer mechanism with significantly larger rate coefficients when a catalyst laser is introduced. The frequency of this catalyst laser is red detuned from the calcium ^{1}S$_0$ to ^{1}P$_1$ laser-cooling transition by hundreds to thousands of natural linewidths. The laser does not excite the Yb$^+$ ion. The left panel of Fig. 5 then shows the relevant CaYb$^+$ dimer potentials with a charge-exchange crossing (CEC) between two of the potentials. The atomic states at the dissociation limit of these potential are shown. Moreover, the difference between the dissociation energies of the two crossing potentials is small compared to the catalyst photon energy. Finally, the figure shows the dressed-state potential for Ca(^{1}S$_0$) + Yb$^+$(^{2}S$_{1/2}$) plus one catalyst photon.

With a quantum coupled-channels calculation based on the potentials in Fig. 5 and their couplings, we then computed the rate coefficient for charge transfer to ionic Ca$^+$(^{2}S$_{1/2}$) and

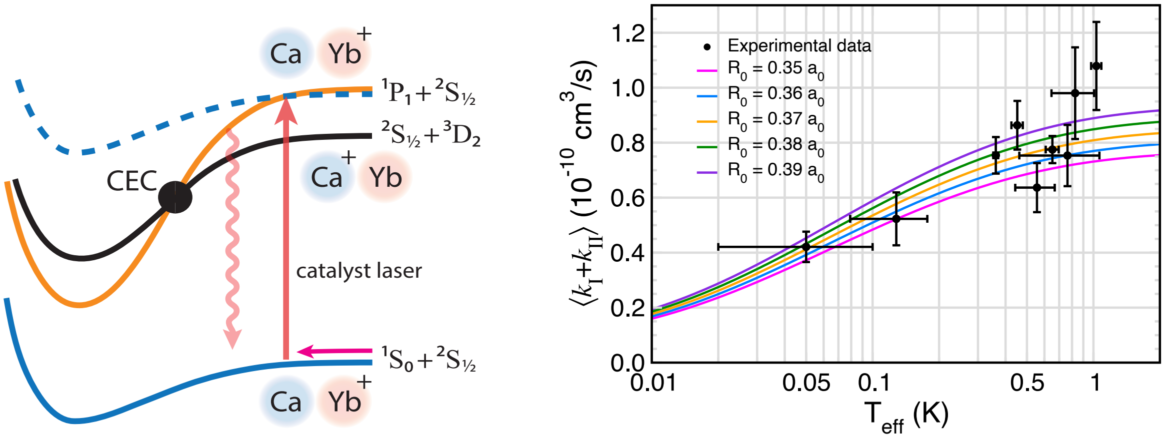

Figure 5: Left panel: Schematic of relevant potentials of the CaYb$^+$ ionic molecule (solid colored curves) as function of atom-ion separation. The catalyst laser excitation pathway is indicated with two straight arrows. The catalyst-photon dressed potential is shown as a dashed curve. The charge-exchange crossing (CEC) between two of the potentials is shown by a black circle. Spontaneous emission (sinusoidal arrow) from the potential dissociating to $\mathrm{Ca}(^1\mathrm{P}_1)+\mathrm{Yb}^+(^2\mathrm{S}_{1/2})$ can occur. Right panel: Total thermalized charge-transfer rate coefficient as a function of the effective temperature T_{eff} in the center-of-mass frame of Ca and Yb$^+$. Filled black circles with one-standard-deviation error bars are experimental data. Solid curves are theoretical predictions with coupling width R_0 ranging from $0.35a_0$ to $0.39a_0$.

electronically-excited neutral $\mathrm{Yb}(^3\mathrm{D}_2)$. For realistic laser intensities large rate coefficients on the order of 10^{-10} cm^3/s were found. Our theoretical rate coefficients as function of temperature are shown in the right panel of Fig. 5 and agreed well with experimental rate-coefficient measurements by the groups of E. Hudson at UCLA. These experimental data are also shown in the figure. A complication in the comparison was that with the small collision energies the atom pair can undergo spontaneous emission before reaching the CEC. This leads to a small suppression of the probability of charge transfer.

We thus showed that the near-degeneracy of the excited asymptotic limits leads to large charge-transfer rate coefficients that can be controlled by changing the frequency of the catalyst laser. Our technique should find use as a general tool for studying excited-state atom-ion charge-exchange reactions.

3 Prospects for laser-induced formation of ultracold molecules

We analyzed the factors that affect the photo-associative creation of LiYb from ultracold fermionic ^{6}Li and ^{173}Yb in the presence of an external magnetic field B. In collaboration with the group of S. Gupta of Washington State University, we located a number of so-called p-wave magnetic Feshbach resonances in collisions of Li and Yb and analyzed the unique temperature dependence of the resonant three-body recombination process through which the resonance was detected. We confirmed that Feshbach resonances in this system are solely the result of a weak separation-dependent hyperfine coupling $\zeta_{\mathrm{Yb}}(R)$ between the electronic spin of ^{6}Li and the nuclear spin of

^{173}Yb. Our analysis also showed that three-body recombination rate coefficients are controlled by the identical fermion nature of the mixture, even when s-wave collisions between Li and Yb are allowed and even when the temperature of the collision falls outside the Wigner threshold regime at our lowest temperature. Specifically, a comparison of experimental and theoretical line shapes of the recombination process indicated that the asymmetric recombination line shape as a function of magnetic field and the temperature dependence of the maximum recombination rate coefficient can only be explained by triatomic collisions with nonzero, p-wave total orbital angular momentum. The resonances can be used to form ultracold doublet $^2\Sigma^+$ ground-state molecules. The locations of the five resonances are shown in Fig. 6(a), whereas Fig. 6(b) shows $\zeta_{\mathrm{Yb}}(R)$ together with the radial wave function of the most weakly-bound state of the $\mathrm{X}^2\Sigma^+$ Born-Oppenheimer potential as a function of interatomic separation R. The $\zeta_{\mathrm{Yb}}(R)$ is on the order of the ^{6}Li atomic hyperfine constant a_{Li} near the inner turning point, $R \approx 6a_0$, of the $\mathrm{X}^2\Sigma^+$ state potential and then approaches zero rapidly when $R \to \infty$.

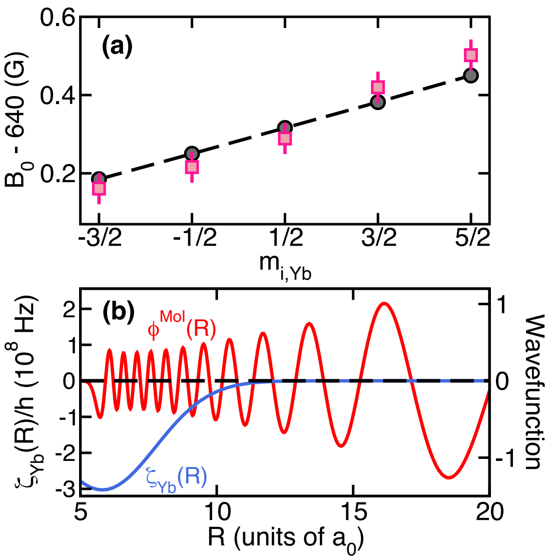

Figure 6: (a) Observed (pink squares) and theoretically predicted (black circles) resonance locations of ^{173}Yb^{6}Li near $B = 640$ G as functions of the ^{173}Yb nuclear spin projection quantum number $m_{i,\mathrm{Yb}}$. (b) The ^{173}Yb^{6}Li hyperfine coupling coefficient $\zeta_{\mathrm{Yb}}(R)$ (solid blue curve) and the radial wave function $\phi^{\mathrm{Mol}}(R)$ of the most weakly-bound state of its $\mathrm{X}^2\Sigma^+$ potential (solid red curve) as functions of separation R.

In separate publications, we studied the formation of ultracold lanthanide molecules using magnetic Feshbach resonances and proposed chemical substitution as a means to engineer large polyatomic molecules with cycling transitions that allow them to be laser cooled to micro-kelvin temperatures.

4 Control of ultracold atoms and molecules in optical traps and lattices

We conclude with briefly mentioning some smaller projects that were helped by funding from the ARO. Quantum gases of ultracold molecules confined in optical potentials require ultimate control of all their degrees of freedom. Our research then included theoretical modeling of dephasing and decoherence processes of ultracold molecules prepared in superpositions of rotational states due to the lasers that hold them in place. In addition, our efforts included spinor-oscillation dynamics of magnetic lanthanide molecules, such as Er_2, and state-dependent trapping schemes for NaK molecules in optical lattices. Finally, we developed a general nondestructive imaging technique for rotational states of ultracold molecules. We described how the anisotropic nature of excited rotational states can lead to a measurable polarization rotation of low-intensity off-resonant probe lasers.

These studies were in part performed in collaboration with the experimental groups of Dr. B. DeMarco and Dr. B. Gadway of the University of Illinois at Urbana-Champaign, USA, Dr. I. Bloch of MPI, Germany, and Dr. J. Ye of JILA, USA.

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Personnel

The following is a list of individuals who have worked part- or full-time on the research supported by the Air Force Office of Scientific Research under Grant FA9550-14-1-0321:

- Prof. S. Kotochigova, Physics Department of Temple University
- C. Makrides, Graduate Student (Ph.D. completed)
- Dr. M. Li, Research Associate, Physics Department of Temple University
- Dr. J. Kłos, Adjunct Professor, Physics Department of Temple University
- Dr. H. Li, Adjunct Professor, Physics Department of Temple University
- C. H. Yuen, Graduate Student (Ph.D. completed)

Invited Talks by PI

1. *Novel states of matter with ultracold magnetic lanthanides*, Colloquium of Physics Department, March 6, 2017, Temple University, PA
2. *Scattering dynamics of ultracold magnetic lanthanides*, NIST Seminar, April 18, 2017, Gaithersburg, MD.
3. *Molecules as reactive species at a collision energy close to absolute zero*, Symposium on "Cold Molecules for Chemistry" at the ACS Spring meeting, March 18-22, 2018, New Orleans, LA.
4. *Chemical Reactions with Ultracold Polar Molecules*, ITAMP International workshop "New frontiers in cold molecules", Cambridge, MA, May 21-23, 2019.
5. *Nonadiabatic Transitions via Conical Intersections in Ultracold Chemical Reactions*, 10th International Society of Theoretical Chemical Physics Tromso, Norway, 11-17 July 2019.
6. *Nonadiabatic Transitions via Conical Intersections at Ultracold Temperatures*, Joint Attosecond Annual Meeting, November 12-22, 2019, Arlington, VA.
7. *Quantum Chemistry with Ulracold Molecule*, Sanibel Symposium, February 18, 2020, Saint Simons Island, GA.
8. *Chemical Reactivity and Nonadiabatic Coupling at Ultralow Temperatures*, United States Naval Academy, Colloquium, Annapolis, January 30, 2020.
9. *Quantum-mechanical studies of interactions with ultracold atoms and molecules*, American Physical Society DAMOP meeting, June 1-5, 2020.
10. *Efficient routes for the cooling radical OH*, American Physical Society, March meeting, March 17, 2021.