

## AUTOPRESENTATION

### I. NAME AND FAMILY NAME

**Michał Tomza**

born on 27 September 1987

### II. DIPLOMAS AND SCIENTIFIC DEGREES

- **Ph.D. degree in Chemistry**

Date: 24 June 2014

Thesis title: *Quantum dynamics and control of ultracold molecules in external fields*

Supervisors: prof. dr. hab. Robert Moszyński and prof. dr. Christiane Koch

Research units: Faculty of Chemistry, University of Warsaw, Poland and Institut für Physik, Universität Kassel, Germany (*cotutelle*)

- **M.Sc. degree in Chemistry**

Date: 4 September 2009

Thesis title: *Two-photon photoassociation of cold atoms in a femtosecond laser field* (in Polish)

Supervisor: prof. dr. hab. Robert Moszyński

Research unit: Faculty of Chemistry, University of Warsaw, Poland

### III. INFORMATION ON PREVIOUS EMPLOYMENT IN SCIENTIFIC INSTITUTIONS

- **Assistant Professor**, since December 2017  
Faculty of Physics, University of Warsaw, Poland
- **Visiting Researcher**, November 2017 – December 2017  
ITAMP, Harvard University, Cambridge, MA, USA
- **Assistant Professor**, November 2016 – November 2017  
Centre of New Technologies, University of Warsaw, Poland
- **Postdoctoral Researcher**, November 2014 – November 2016  
ICFO - Institut de Ciències Fotòniques, Barcelona, Spain
- **Visiting Postdoctoral Researcher**, October 2014  
JILA, University of Colorado at Boulder, CO, USA
- **Postdoctoral Researcher**, July 2014 – August 2014  
University of British Columbia, Vancouver, Canada
- **Ph.D. Student**, April 2011 – June 2014  
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IV. INDICATION OF THE ACHIEVEMENT ACCORDING TO ART. 16 ACTS OF LAWS ON ACADEMIC DEGREES FROM 14.03.2003 (Dz. U. 2016 r. poz. 882 ze zm. w Dz. U. z 2016 r. poz. 1311.):

A. TITLE OF THE SCIENTIFIC ACHIEVEMENT

A series of articles entitled:

*Interactions and collisions between ultracold atoms, ions, and molecules*

B. LIST OF PUBLICATIONS FORMING THE SCIENTIFIC ACHIEVEMENT  
(reverse chronological order)

- [H1] L. Tanzi, C. R. Cabrera, J. Sanz, P. Cheiney, **M. Tomza**, L. Tarruell, *Feshbach resonances in potassium Bose-Bose mixtures*, Physical Review A 98, 062712 (2018).
- [H2] K. Zaremba-Kopczyk, P. S. Żuchowski, **M. Tomza**, *Magnetically tunable Feshbach resonances in ultracold gases of europium atoms and mixtures of europium and alkali-metal atoms*, Physical Review A 98, 032704 (2018).
- [H3] A. Dawid, M. Lewenstein, **M. Tomza**, *Two interacting ultracold molecules in a one-dimensional harmonic trap*, Physical Review A 97, 063618 (2018), Highlighted as Editors' Suggestion.
- [H4] T. Schmid, C. Veit, N. Zuber, R. Löw, T. Pfau, M. Tarana, **M. Tomza**, *Rydberg molecules for ion-atom scattering in the ultracold regime*, Physical Review Letters 120, 153401 (2018).
- [H5] H. FÜRST, T. Feldker, N. Ewald, J. Joger, **M. Tomza**, R. Gerritsma, *Dynamics of a single ion spin impurity in a spin-polarized atomic bath*, Physical Review A 98, 012713 (2018).
- [H6] J. Joger, H. FÜRST, N. Ewald, T. Feldker, **M. Tomza**, R. Gerritsma, *Observation of collisions between cold Li atoms and Yb<sup>+</sup> ions*, Physical Review A 96, 030703(R) (2017), Rapid Communication.
- [H7] **M. Tomza**, *Cold interactions and chemical reactions of linear polyatomic anions with alkali-metal and alkaline-earth-metal atoms*, Physical Chemistry Chemical Physics 19, 16512 (2017).
- [H8] B. Midya, **M. Tomza**, R. Schmidt, M. LEMESHKO, *Rotation of cold molecular ions inside a Bose-Einstein condensate*, Physical Review A 94, 041601(R) (2016), Rapid Communication.
- [H9] **M. Tomza**, *Ultracold magnetically tunable interactions without radiative charge transfer losses between Ca<sup>+</sup>, Sr<sup>+</sup>, Ba<sup>+</sup>, and Yb<sup>+</sup> ions and Cr atoms*, Physical Review A 92, 062701 (2015).
- [H10] **M. Tomza**, *Energetics and control of ultracold isotope-exchange reactions between heteronuclear dimers in external fields*, Physical Review Letters 115, 063201 (2015).

Detailed information about my contribution to the articles above is collected in Załącznik nr 4 (Appendix 4).

## C. DESCRIPTION OF THE SCIENTIFIC ACHIEVEMENT

The cold and ultracold synthetic systems attract great interest because the quantum nature of the world is visibly manifested at ultralow temperatures, that is temperatures below 1 miliKelvin, and research on such systems gives a new insight into the quantum theory of matter and matter-light interactions [1–3]. In this context, all ten articles [H1]-[H10], which constitute the presented achievement, describe interactions and collisions between ultracold atoms, ions, and molecules, together with potential applications and implications for contemporary experimental works. In fact, the articles [H1], [H5], and [H6] present joined experimental and theoretical results, where the developed theory guided and helped to interpret experimental efforts. The article [H4] is a theoretical proposal intended to guide ongoing experimental work and the articles [H2], [H3], [H7], [H8], [H9], and [H10] propose and analyze in detail new ultracold systems ready to be implemented in modern experiments in the near future. In all articles, special attention is paid to take into account experimental possibilities and technical limitations.

The subjects of the presented articles overlap and complement each other on several levels, including used theoretical methods, physical implementations, and experimental implications, but the following four largest categories can be distinguished:

- ultracold ion-atom systems: [H4], [H5], [H6], [H7], [H8], [H9],
- ultracold molecular systems: [H3], [H4], [H7], [H8], [H10],
- quantum control of ultracold systems: [H1], [H2], [H3], [H4], [H4], [H5], [H6], [H10],
- magnetically tunable Feshbach resonances: [H1], [H2], [H5], [H9].

The structure of this part of the autopresentation is as follows. Section 1 is an introduction to the field of ultracold atoms, ions, and molecules. Section 2 describes theoretical methods used in the presented series of articles. Section 3 presents results of the articles [H1]-[H10]. The last section 4 summarizes the presentation.

Additionally, I encourage the reader to become familiar with the review article on *Cold hybrid ion-atom systems* [O1], which covers significant part of theoretical methods and systems used and presented in the articles [H1]-[H10]. The review article was prepared under my supervision and with my dominant contribution, and is accepted for publication in *Reviews of Modern Physics*.

### 1. Introduction to ultracold atom, ions, and molecules

The development of laser and cooling techniques resulted in the birth and successful advances of the field of cold and ultracold matter in recent decades [4, 5]. Ultracold gases are ideal systems for engineering highly nontrivial states of matter, and thus for quantum simulation and precision measurements, because they allow one to prepare, manipulate, and measure with great accuracy strongly interacting quantum systems [6–9]. After many spectacular successes in the research on ultracold atoms, the scientific community has recently drawn its attention to the research on ultracold molecules, Rydberg atoms, ions, and their mixtures with ultracold atoms. Such mixtures possess a richer internal structure as compared to atoms thus promising new exciting applications [10–12].

Ultracold trapped atoms and polar molecules are fascinating and likely useful systems which interactions, structure, and geometry can potentially be controlled over a wide range of parameters. They can be used to simulate a plethora of quantum phenomena relevant for condensed matter physics by mimicking the behavior of systems of interest. The first quantum simulations of fundamental quantum phenomena with ultracold atoms in optical lattices were already demonstrated [8, 13–16]. Ultracold polar molecules in optical lattices were proposed for the realization

of dipolar quantum phases [17] and spin models [18], the simulation of the condensed-matter physics [8] or quasi-particles [19], the implementation of quantum computing [20], the precision measurements [21, 22], and many others [10]. The production of the high phase-space-density gases of ultracold molecules [23–28] have allowed for groundbreaking experiments on controlled chemical reactions [29–32]. The reduction of ultracold molecular gas dimensionality [33] and the observation of dipolar spin-exchange interactions between lattice-confined polar molecules [34] have opened the way to the quantum simulation of exotic quantum phases and other phenomena of quantum many-body physics.

Trapped atomic ions are highly controllable systems with strong interactions and thus find many applications, for example in precision measurements, quantum simulation, quantum computing, and quantum metrology [35–37]. The development of the laser cooling of trapped atomic ions to their motional ground state [38] opened the way to the ground-breaking experiments on measurement and manipulation of individual quantum systems. The theoretical proposal of Ignacio Cirac and Peter Zoller in 1995 suggested that the quantum computer can be implemented with cold atomic ions confined in a linear ion trap and interacting with laser beams [39]. This proposal boosted the research on laser-cooled trapped atomic ions. The quantum simulations of the fundamental quantum logic gate [40], the Cirac–Zoller controlled-NOT quantum gate [41], the entangled states [42], the Dirac equation [43], the open quantum systems [44], the implementation of the Deutsch–Jozsa algorithm [45], the repetitive quantum error correction [46], the universal digital quantum simulator [47], the scalable Shor algorithm [48], and many others were realized with trapped atomic ions.

An atom excited to the Rydberg state has enormously large electric dipole polarizability ( $\sim n^7$ , where  $n$  is the principal quantum number) due to the weak binding and extremely large size ( $\sim n^2$ ) of the Rydberg electron orbital [49]. This huge polarizability results in very strong interatomic interactions of the van der Waals or dipole-dipole type between two atoms excited to Rydberg states. These very strong interactions can be employed to control ultracold collisions between atoms. For example, the first fast quantum gates for neutral atoms were proposed using this technique [50]. The strong and long-range interactions between atoms in the Rydberg state, which shift the energy levels, result also in other genuine phenomenon of the Rydberg excitation blockade, which suppresses the possibility of exciting two nearby atoms at the same time [51, 52]. Therefore, the atomic Rydberg systems find many applications in manipulating photon states in atomic ensembles [53], as well as quantum simulation of many-body physics [54] and quantum computing [55]. The first quantum simulators based on Rydberg excitations in atom-by-atom assembled systems were also realized [56, 57]. Other interesting research direction is the formation of ultralong-range Rydberg molecules [58, 59]. Thus, quantum mixtures of atoms with Rydberg atoms have very interesting and varied nature.

Recently, hybrid systems of laser-cooled trapped ions and ultracold atoms combined in a single experimental setup have emerged as a new platform for fundamental research in quantum physics and chemistry [60]. These systems combine the best features of the two well-established fields: trapped ions [38] and ultracold atoms [7]. The ion can be trapped in the Paul trap, but the minimal feasible energy of ion-atom collisions in this trap is limited to several  $\mu\text{K}$  by micromotion induced by rf frequency [61, 62]. Fortunately, the dipole traps for ions have also been developed opening the way to ultracold ion-atom systems [63–65]. Their potential applications range from cold controlled ion-atom collisions and chemical reactions [66–69] to quantum simulation of solid-state physics [70, 71] and quantum computing [72]. Cold molecular ions can be formed from cold mixtures of atomic ions and atoms [O4], or they can be cooled down from room temperature using laser, buffer-gas, or sympathetic cooling [73–75]. Potential applications of molecular ions include precision measurements [76, 77], cold controlled chemistry [78, 79], and novel quantum simulation. The first experiments combining simple diatomic molecular ions with ultracold atoms have also been recently launched.

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## 2. Research methodology

The research, which constitutes the presented achievement, aimed at the development of new concepts, methods, and tools for theoretical and experimental studies of ultracold quantum mixtures of atoms, ions, and molecules – the systems, which are interesting from the fundamental point of view, yet not well explored. To obtain planned goals, we used the state-of-the-art methods of molecular physics and quantum chemistry, as well as developed new programs, models, and theoretical methods when it was needed.

Potential energy curves, transition electric dipole moments, and spin-orbit coupling matrix elements for selected molecular systems were calculated using state-of-the-art *ab initio* methods of quantum chemistry accounting for both static and dynamic correlation energy and relativistic effects [80, 81]. To investigate the electronic structure of closed-shell and high-spin (spin-stretched) open-shell systems in the ground state, we used the coupled cluster method restricted to single, double, and noniterative triple excitations, CCSD(T) [82, 83]. The transition electric dipole moments were also calculated with coupled cluster methods, if possible, e.g. using the linear response theory within the coupled cluster singles and doubles framework [81]. In all other cases, especially for transition electric dipole moments and spin-orbit coupling matrix elements, we employed the multireference configuration interaction method restricted to single and double excitations, MR-CISD [84]. Electronic structure calculations were performed with the MOLPRO package of *ab initio* programs [85].

The interaction energies were obtained with the supermolecule method with the basis set superposition error corrected by using the counterpoise correction [86]  $V_{A+B} = E_{A+B} - E_A - E_B$ , where  $E_{A+B}$  denotes the total energy of the interacting complex, and  $E_A$  and  $E_B$  are the total energies of the monomers computed in the dimer basis set. In all calculations we used large basis sets and large active spaces, and the results were extrapolated to the complete basis set limit, when possible. Light atoms were described by the augmented correlation consistent Dunning's basis sets (aug-cc-pVnZ) with the  $n$  between 3 and 5. Other alkali-metal and alkaline-earth-metal atoms were described with the small-core relativistic energy-consistent pseudopotentials (ECP) to replace the inner-shells electrons [87]. Thus, we treated heavy alkali-metal and alkaline-earth-metal atoms as systems of effectively 9 and 10 electrons, respectively. They were described with the basis sets obtained by taking the basis sets suggested by the authors of pseudopotentials but augmented and optimized by us in previous projects [O14,O10,O8,O7]. The scalar relativistic effects on heavy atoms were included by used pseudopotentials. The employment of the pseudopotentials allowed us to use larger basis sets to describe the valence electrons and to model the inner-shells electrons density as accurately as the high quality atomic calculation used to fit pseudopotentials. The pseudopotentials from the Stuttgart library were employed in all calculations [87].

The long-range interaction coefficients, which are especially crucial for cold physics and chemistry, were obtained using the perturbation theory [88]. The interaction potential between an atomic ion and an atom, both in the electronic ground state without orbital angular momentum, at large intermolecular distances  $R$ , in the body-fixed frame, reads

$$V(R) = -\frac{C_4^{\text{ind}}}{R^4} - \frac{C_6^{\text{ind}}}{R^6} - \frac{C_6^{\text{disp}}}{R^6} + \dots, \quad (1)$$

where the leading long-range induction coefficients are  $C_4^{\text{ind}} = \frac{1}{2}q^2\alpha_{\text{atom}}$  and  $C_6^{\text{ind}} = \frac{1}{2}q^2\beta_{\text{atom}}$ , where  $\alpha_{\text{atom}}$  is the static electric dipole polarizability of the atom,  $q$  is the charge of the ion, and  $\beta_{\text{atom}}$  is the static electric quadrupole polarizability of the atom. The leading long-range dispersion coefficient is  $C_6^{\text{disp}} = \frac{3}{\pi} \int_0^\infty \bar{\alpha}_{\text{ion}}(i\omega)\bar{\alpha}_{\text{atom}}(i\omega)d\omega$ , where  $\alpha_{\text{atom/ion}}(i\omega)$  is the dynamic polarizability of the atom/ion at imaginary frequency. If an atom has a more complex structure and possesses non-zero orbital angular momentum, then additional terms appear in Eq. (2), such as  $-C_3^{\text{elst}}/R^3$  and  $-C_5^{\text{elst}}/R^5$  that describe

the long-range charge-quadrupole and charge-hexadecapole interactions [89], respectively. The two leading terms of the long-range interaction potential between a diatomic molecular ion and an atom are

$$V(R, \theta) = -\frac{C_4^{\text{ind}}}{R^4} - \frac{C_5^{\text{ind}}}{R^5} \cos \theta + \dots, \quad (2)$$

where  $C_5^{\text{ind}} = 2\alpha_{\text{atom}} q d_{\text{ion}}$ , where  $d_{\text{ion}}$  is the dipole moment of the molecular ion.

The static electric properties of monomers were calculated using the finite field method combined with suitable quantum-chemical methods. The dynamic polarizabilities at imaginary frequency were either taken from previous accurate atomic calculations (e.g. Ref. [90] for alkali-metal and alkaline-earth-metal atoms) or obtained by using the explicitly connected representation of the expectation value and polarization propagator within the coupled cluster method [91, 92] for closed-shell species and the sum-over-states formalism for open-shell ones.

The nuclear dynamics of two colliding species was described by solving the Schrödinger equation with corresponding Hamiltonian for the nuclear motion. The general Hamiltonian describing the relative nuclear motion of the  $A$  atom and the  $B$  atom is of the form [O4,O5]

$$\hat{H} = -\frac{\hbar^2}{2\mu} \frac{1}{R} \frac{d^2}{dR^2} R + \frac{\hat{L}^2}{2\mu R^2} + \sum_{S, M_S} V_S(R) |S, M_S\rangle \langle S, M_S| + V^{ss}(R) + \hat{H}_A + \hat{H}_B, \quad (3)$$

where  $\mu$  is the reduced mass,  $R$  is the internuclear distance,  $\hat{L}$  is the rotational angular momentum operator, and  $V_S(R)$  is the potential energy curve for the state with total electronic spin  $S$ .  $V^{ss}(R)$  is the spin-dipole–spin-dipole interaction responsible for the dipolar relaxation [93]. The atomic Hamiltonian,  $\hat{H}_j$  ( $j = A, B$ ), including Zeeman and hyperfine interactions, is given by

$$\hat{H}_j = \zeta_j \hat{i}_j \cdot \hat{s}_j + (g_e \mu_B \hat{s}_{j,z} + g_j \mu_N \hat{i}_{j,z}) B_z \quad (4)$$

where  $\hat{s}_j$  and  $\hat{i}_j$  are the electron and nuclear spin operators,  $\zeta_j$  is the hyperfine coupling constant,  $g_{e/j}$  are the electron and nuclear  $g$  factors, and  $\mu_{B/N}$  are the Bohr and nuclear magnetons.

The bound ro-vibrational states for Hamiltonian (3) were calculated using exact diagonalization with discrete variable representation with intermolecular distance represented on a Fourier grid with an adaptive step size [94–96] and spin and angular degrees of freedom represented in a properly symmetrized basis of spherical harmonics. Calculated eigenstates were used to evaluate the Franck-Condon factors and Einstein coefficients.

The scattering states and properties were calculated using the scattering code written in Fortran 95. The total scattering wave functions were constructed in a fully uncoupled basis set assuming the projection of the total angular momentum to be conserved. The non-adiabatic (beyond Born-Oppenheimer approximation) calculations on several electronic states coupled by hyperfine structure were realized. The basis set functions were products of eigenstates associated with the angular momenta present in the system (e.g. electronic and nuclear spins, end-over-end rotation, molecular rotation). The coupled-channel equations were solved using the renormalized Numerov propagator [97] with step-size doubling. The wave function ratios were propagated to large intermolecular separations, transformed to the diagonal basis, and the  $K$  and  $S$  matrices were extracted by imposing the long-range scattering boundary conditions in terms of the Bessel functions. The scattering lengths, elastic, inelastic, and reactive cross sections were obtained from the  $S$  matrix.

The time evolution for time-independent Hamiltonians was realized by propagation in the diagonal basis of eigenstates obtained in the exact diagonalization. The time evolution for time-dependent Hamiltonians with time-dependent control fields was studied with the split operator and Chebyshev propagator [98].

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### 3. Description of obtained results

#### Feshbach resonances in potassium Bose-Bose mixtures

Magnetically tunable Feshbach resonances are a universal and useful tool to control collisional properties in ultracold quantum gases [99, 100]. Over the last 20 years, they have enabled the study of a wealth of few- and many-body phenomena. Key examples include the magneto-association of ultracold Feshbach molecules [101], the observation of Efimov bound states [102] and the study of strongly-interacting systems, a prime example of which are unitary limited gases [103].

In the article [H1], in collaboration with the experimental group of Prof. Leticia Tarruell at the Institute of Photonic Science in Barcelona, we performed a comprehensive experimental and theoretical study of the low energy scattering properties of various potassium Bose-Bose mixtures. We located 20 previously unobserved Feshbach resonances in the mixture  $^{39}\text{K}$ - $^{41}\text{K}$ , and confirmed the validity of the model potentials proposed in Ref. [104] for this isotopic combination. Exemplary comparison of obtained experimental and theoretical results is presented in Fig. 1. At the level of accuracy of experiment and theory, this constituted a test of the validity of the Born-Oppenheimer approximation for potassium scattering. For  $^{41}\text{K}$  we identified a new interstate Feshbach resonance that gives access to two-component Bose gases with repulsive intrastate interactions and tunable interstate ones. For  $^{39}\text{K}$  we measured the binding energy of the molecular state responsible for the interstate Feshbach resonance at  $\sim 114$  G [105]. Combining experimental observations, quantum calculations and analytical models, we provided a precise characterization of the resonance parameters, including the resonance strength and its range parameter. The model employed to analyze this specific resonance incorporated explicit calculations of the field-dependent effective range and background scattering length and accounts for non-universal finite-range effects. Due to its simplicity, this model could be used to characterize other Feshbach resonances.

The 23 Feshbach resonances characterized in this work could be exploited to improve the model potentials for potassium scattering. Such efforts should include as well the new  $^{40}\text{K}$  [106],  $^{41}\text{K}$  [107] and  $^{40}\text{K}$ - $^{41}\text{K}$  resonances [108] that have been located during the last years, and the most recent measurements on single-component  $^{39}\text{K}$  gases [109, 110]. Furthermore, the tunability of scattering lengths available in potassium Bose-Bose mixtures opens a wealth of possibilities for future research. The  $^{39}\text{K}$ - $^{41}\text{K}$  mixture enables the realization of three-component Bose gases with tunable interactions, where magnetic polarons have been predicted [111]. In the presence of coherent coupling, the  $^{41}\text{K}$  interstate resonance is well suited for the study of the paramagnetic-ferromagnetic phase transition, and for adding interaction control to experiments with synthetic gauge fields in synthetic dimensions [112–114]. Finally, the  $^{39}\text{K}$  interstate resonance constitutes an ideal system for the observation of Bose

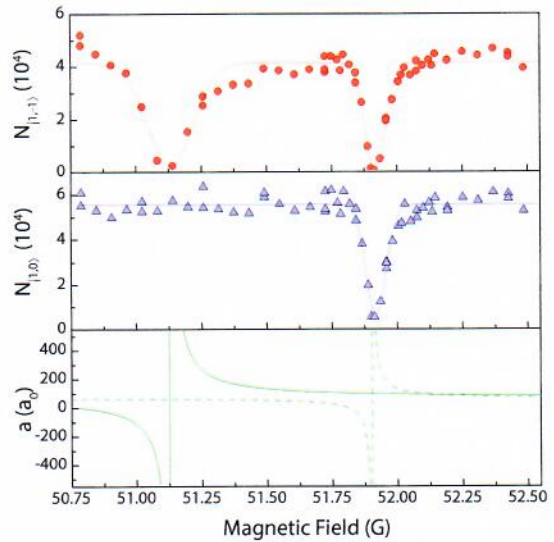


Figure 1: Feshbach resonances for  $^{41}\text{K}$  collisions in the  $|1, -1\rangle + |1, -1\rangle$  and  $|1, 0\rangle + |1, -1\rangle$  scattering channels. Top and middle panels: experimentally observed loss features for the  $|1, -1\rangle$  (red circles) and  $|1, 0\rangle$  (blue triangles) states. The solid line is the empirical Gaussian fit used to extract the resonance positions. Bottom panel: scattering lengths for  $|1, -1\rangle + |1, -1\rangle$  (continuous line) and  $|1, -1\rangle + |1, 0\rangle$  (dashed line) collisions predicted by our CC calculations. The  $|1, 0\rangle + |1, 0\rangle$  scattering length does not vary in this magnetic field range, and remains close to the background value  $\sim 65a_0$ . From the article [H1].

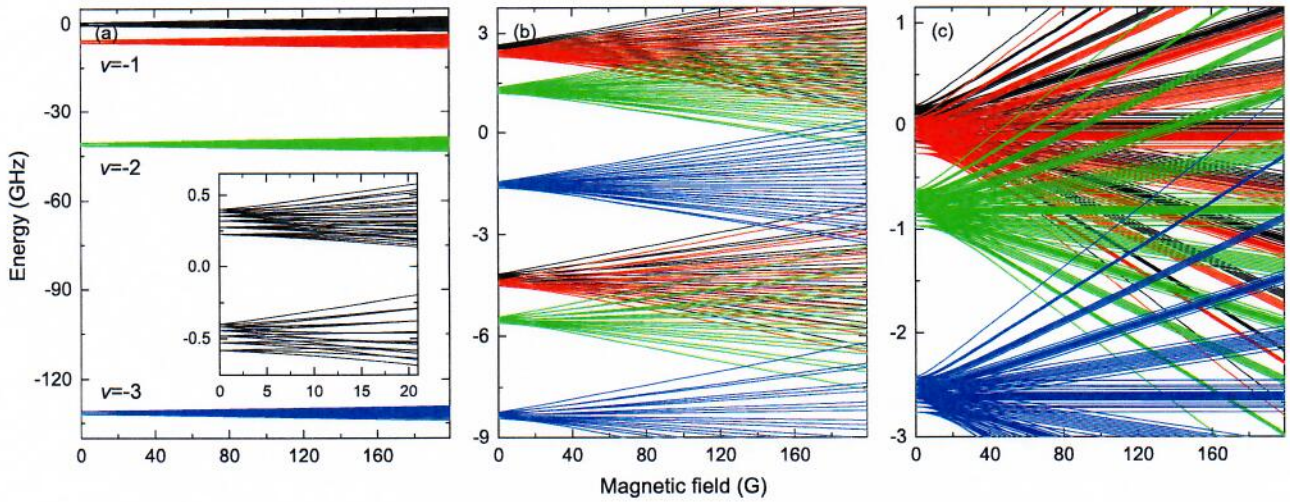


Figure 2: Hyperfine energy levels for mixtures of (a)  $^{153}\text{Eu}+^7\text{Li}$ , (b)  $^{153}\text{Eu}+^{87}\text{Rb}$ , and (c)  $^{153}\text{Eu}+^{151}\text{Eu}$  atoms with the projection of the total angular momentum  $M_{\text{tot}} = 0$  as a function of the magnetic field. Black lines show atomic thresholds, whereas colorful lines correspond to the progression of the last three most weakly bound vibrational molecular levels for infinitely large and negative scattering lengths. From the article [H2].

polarons in the strongly interacting regime [105]. The presented study of Feshbach resonances was essential for the realization of quantum liquid droplets in a mixture of Bose-Einstein condensates in the group of Prof. Tarruell [115, 116].

### Feshbach resonances in ultracold gases of Eu atoms and mixtures of Eu and alkali-metal atom

Magnetic Feshbach resonances are expected between any open-shell atoms, but first applications involved ultracold alkali-metal atoms [117]. Nevertheless, they were also observed and employed in experiments with ultracold Cr atoms [118–122], and recently with ultracold Er and Dy atoms [123–129]. Ultracold gases of dipolar atoms are especially interesting because the rich physics of different quantum phases and spin models can be realized with them [130, 131]. Therefore, atoms in complex electronic states with large both spin and orbital electronic angular momenta, such as Er and Dy, have been cooled down to low and ultralow temperatures. Tremendous successes have already been accomplished with these atoms, just to mention the observation of quantum chaos in ultracold collisions [132], Fermi surface deformation [133], self-bound quantum droplets [134], Rosensweig instability [135], and extended Bose-Hubbard models [136]. The spin dynamics of impurities in a bath of strongly magnetic atoms and magnetic polaron physics [111, 137] wait for realization.

Dy and Er atoms are excellent systems for experiments exploiting dipolar interactions, but their very complex internal structure resulting in very rich, dense, and chaotic spectra of unavoidable magnetic Feshbach resonances [129] can limit applications based on the precision control of internal degrees of freedom, such as magnetoassociation, optical stabilization to deeply bound states, or magnetic polaron physics investigations. The use of ultracold Eu atoms may be a remedy. Therefore, in the article [H2], we considered ultracold collisions involving Eu atoms as another lanthanide candidate for the realization and application of dipolar atomic and molecular quantum gases in many-body physics. We investigated magnetically tunable Feshbach resonances between ultracold europium atoms and between europium and alkali-metal atoms using multichannel quantum scattering calculations. For ultracold gases of europium atoms both homonuclear  $^{153}\text{Eu}+^{153}\text{Eu}$  and heteronuclear  $^{151}\text{Eu}+^{153}\text{Eu}$  systems were studied. Calculations for mixtures of europium and alkali-metal atoms were carried out for prototype systems of  $^{153}\text{Eu}+^{87}\text{Rb}$  and  $^{153}\text{Eu}+^7\text{Li}$ . Hyperfine energy



levels for those mixtures are presented in Fig. 2. We analyzed the prospects for the control of scattering properties, observation of quantum chaotic behavior, and magnetoassociation into ultracold polar and paramagnetic molecules. We showed that favorable resonances can be expected at experimentally feasible magnetic field strengths below 1000 G for all investigated atomic combinations. For Eu atoms, a rich spectrum of resonances is expected as a result of the competition between relatively weak short-range spin-exchange and strong long-range magnetic dipole-dipole interactions, where the dipolar interaction induces measurable resonances. A high density of resonances is expected at magnetic field strengths below 200 G without pronounced quantum chaos signatures. The present results may be useful for the realization and application of dipolar atomic and molecular quantum gases based on europium atoms in many-body physics.

## Two interacting ultracold molecules in a one-dimensional harmonic trap

Recently, the deterministic preparation of tunable few-fermion systems with complete control over the number of particles, and their quantum state has become possible [138], opening the way towards quantum simulation of strongly correlated few-body systems. The fermionization of two distinguishable fermions [139], formation of a Fermi sea [140], pairing in few-fermion systems [141], antiferromagnetic Heisenberg spin chain [142], and two fermions [143] or bosons [144, 145] in a double well have been experimentally investigated in 1D. On the other hand, the atom-by-atom assembling of defect-free 1D and 2D cold atom arrays has also been realized [56, 57]. In this way the production of fully controllable synthetic quantum matter can be achieved using both top-down and bottom-up approaches.

Experimental possibilities have motivated intensive theoretical studies of few-body atomic systems. Ultracold molecules have a much richer internal structure as compared to atoms [10]. This includes rotational and vibrational levels together with possible permanent electric dipole moment. Recently, the first step towards atom-by-atom assembled few-body molecular systems has been taken [146] and optical tweezers have been used to assemble and control molecules at the single particle level [147]. All above developments pave the way towards the realization and application of a bottom-up molecule-by-molecule assembled molecular quantum simulator.

In the article [H3], we investigated a fundamental building block of such a simulator, that is two interacting polar molecules effectively trapped in a one-dimensional harmonic potential (see Fig. 3). In our model we described molecules as distinguishable rigid quantum rotors, which interact in a one-dimensional harmonic trap *via* a multichannel two-body contact potential incorporating short-range isotropic and anisotropic intermolecular interactions. We analyzed in detail the properties of such systems including the interplay of the molecular rotational structure, anisotropic interactions, spin-rotation coupling, external electric and magnetic fields, and harmonic trapping potential. Energy spectra and eigenstates were calculated by means of the exact diagonalization.

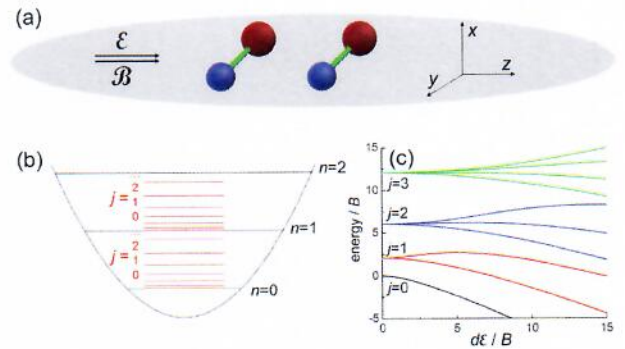


Figure 3: Schematic representation of the investigated system and its features: (a) Illustration of two diatomic polar molecules in a 1D trap in external electric  $\mathcal{E}$  and magnetic  $\mathcal{B}$  fields. (b) The energy spectrum of a rotating molecule in a 1D harmonic trap. (c) The energy of a polar molecule in an electric field (Stark's effect). From the article [H3].

We carefully applied several approximations needed to simplify calculations, and to separate the impact and importance of different features of the molecular structure and intermolecular interactions on the system's dynamics. We investigated the properties of such a system in a broad range of system's parameters and external fields strengths. Our calculations may be considered as a microscopic model for the on-site interaction of the molecular multichannel Hubbard Hamiltonian [148–150] and may provide underlying parameters for effective molecular many-body Hamiltonians. We showed that the anisotropic intermolecular interaction brings states with higher total rotational angular momenta to lower energies such that the absolute ground state of the molecular system can have the total angular momentum larger than zero and be degenerate (see Fig. 4). Such systems may potentially be useful for realizing quantum simulators of exotic spin models. A strong anisotropic intermolecular interaction can induce the emergence of the molecular equivalent of the atomic super-Tonks-Girardeau limit but, at the same time, the importance of the anisotropic intermolecular interaction is reduced in the limit of a very strong isotropic interaction. Magnetic and electric fields induce a high density of states and a large number of avoided crossings, which can be used to control system's properties. No signatures of quantum chaotic behavior in energy spectra was, however, found.

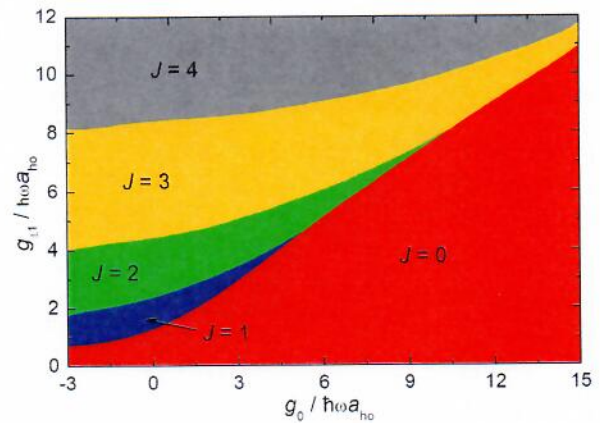


Figure 4: Total rotational angular momentum  $J$  of the ground state for two interacting molecules with the rotational constant  $B = 0.3\hbar\omega$  in a one-dimensional harmonic trap as a function of the isotropic  $g_0$  and anisotropic  $g_{\pm 1}$  interaction strengths. From the article [H3].

### Rydberg molecules for ion-atom scattering in the ultracold regime

In the past few years, the ion-atom interactions could be studied down to the millikelvin regime for various ion-atom combinations by the use of hybrid traps, with the ion held in a Paul trap [O1]. However, the ultracold, quantum scattering regime could not be reached yet. It was shown [62] that by the use of a Paul trap there arises a micromotion-induced limit on the minimum collision energy which can be reached. Only for a combination of a heavy ion with a light atom, e.g., the  $\text{Ca}^+$  - Li or the  $\text{Yb}^+$  - Li system, might the  $s$ -wave collision regime be entered. For both of these ion-atom combinations, collision measurements have recently been carried out in the millikelvin energy range [151][H6] which was, however, still in the classical regime.

In the article [H4], in collaboration with the experimental group of Prof. Tillman Pfau at the University of Stuttgart, we proposed a novel experimental method to extend the investigation of ion-atom interactions from the hitherto studied cold regime to the unexplored ultracold regime. The key aspect of this method was the use of Rydberg molecules to initialize the ultracold ion-atom scattering event. The generation and characterization of many different types of Rydberg molecules have been an active area of research in the past few years. These molecules consist of a Rydberg atom and at least one ground state atom which is bound to the Rydberg ionic core at a very large internuclear distance via its attractive interaction with the Rydberg electron [58]. Triplet  $S$ -state Rydberg dimers, trimers, tetramers, and pentamers have been observed [59, 152, 153], and molecular lifetimes have been measured [154, 155]. Furthermore, triplet  $D$ -state dimers have been studied [156, 157] as well as mixed singlet-triplet dimers [158, 159]. Finally, trilobite [160–163] and butterfly [164] molecules have been investigated.

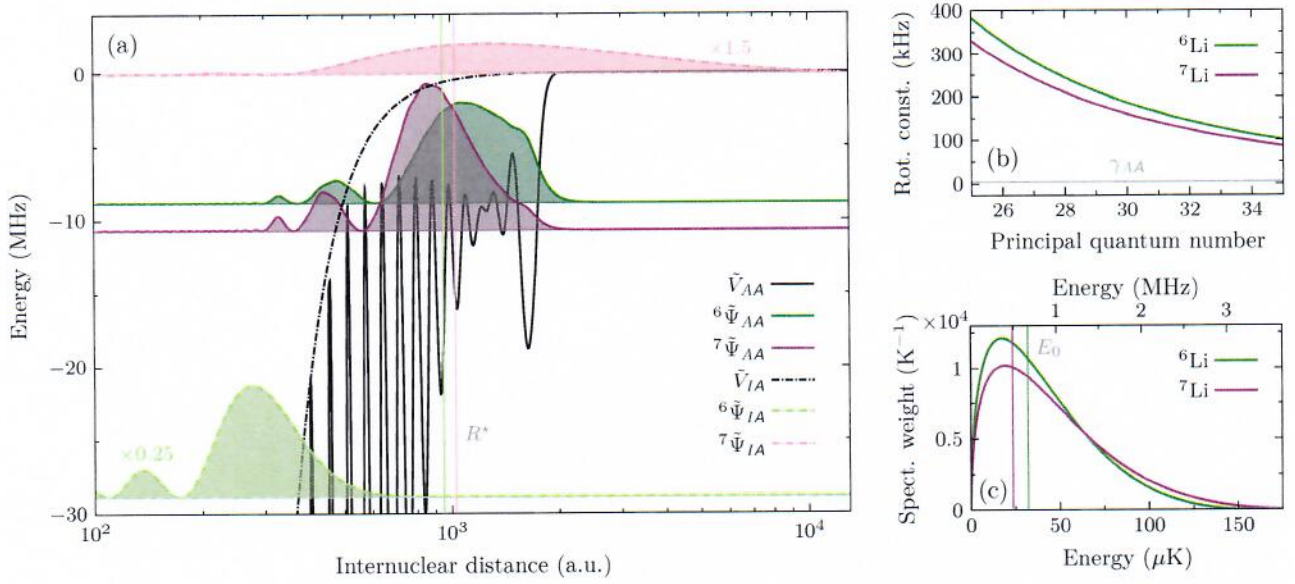


Figure 5: Using Rydberg molecules to initialize an ultracold ion-atom scattering event, exemplified with lithium. The Rydberg molecule wave function of interest, more precisely,  $R^2 |\Psi_{AA}(R)|^2$ , is shown in (a) for both isotopes. It is bound in the homonuclear Li(30s) - Li(2s) potential  $\tilde{V}_{AA}(R)$ . It is in its spherically symmetric rovibrational ground state ( $\tilde{\nu} = \tilde{j} = 0$ ), which can be experimentally addressed, evident from (b), as the rotational constant is larger than the Rydberg molecule decay linewidth  $\gamma_{AA}$ . Freed by photoionization, the initial Rydberg molecule wave function evolves in the spherically symmetric ion-atom interaction potential  $\tilde{V}_{IA}(R)$ , with  $R^*$  denoting its characteristic radius. Because of angular momentum conservation, only S-wave scattering occurs ( $\tilde{j} = 0$ ) despite the components above  $E_0$  in the Rydberg molecule energy spectrum; see (c). The overlap between  $\tilde{\Psi}_{AA}$  and the last bound molecular ion wave function  $\tilde{\Psi}_{IA}$  [see (a)] determines the bound fraction in the scattered wave packet. From the article [H4].

The starting point of the proposed procedure is the photoassociation of a single Rydberg molecule in an ultracold, dilute atomic cloud. The Rydberg molecule is then photoionized to start the ultracold ion-atom scattering event between the Rydberg ionic core and the ground state atom; i.e., the initial Rydberg molecule wave function, freed by photoionization, evolves in the presence of the ion-atom scattering potential. Depending on the scattering length, either the entire scattered wave packet is free and dispersively expanding, or it splits into a free part and a bound part, indicating the formation of a molecular ion. The detection of the free ion and/or the molecular ion with a time- and position-sensitive single-ion detector concludes the single ultracold ion-atom scattering event. The frequent repetition of this single scattering event eventually allows for the determination of the ion-atom scattering length. We exemplified the proposed method with the lithium ion-atom system, for which we presented simulations of how the initial Rydberg molecule wave function, freed by photoionization, evolves in the presence of the ion-atom scattering potential. We predicted bounds for the ion-atom scattering length from *ab initio* calculations of the interaction potential. We demonstrated that, in the predicted bounds, the scattering length can be experimentally determined from the velocity of the scattered wave packet in the case of  ${}^6\text{Li}^+ - {}^6\text{Li}$  and from the molecular ion fraction in the case of  ${}^7\text{Li}^+ - {}^7\text{Li}$ . The proposed method to utilize Rydberg molecules for ultracold ion-atom scattering, here particularized for the lithium ion-atom system, is readily applicable to other ion-atom systems as well, e.g., to homo- or heteronuclear alkali or alkaline earth ion-atom systems for which Rydberg molecules can be formed.

## Mixtures of laser-cooled $\text{Yb}^+$ ions and ultracold fermionic Li atoms

A major roadblock towards reaching the quantum regime in ion-atom interactions is formed by the time-dependent trapping field of the Paul trap, which limits attainable temperatures in hybrid ion-atom systems [O1]. In particular, the micromotion of ions trapped in radio frequency traps may induce heating when short-range (Langevin) collisions with atoms occur. It was shown theoretically that the lowest temperatures may be reached for the largest ion/atom mass ratios  $m_i/m_a$  [62]. The ion-atom combination with the highest mass ratio,  $m_i/m_a \approx 24\text{--}29$  which allows for straightforward laser cooling is  $\text{Li}\text{--}\text{Yb}^+$ . This combination reaches the  $s$ -wave limit at a collision energy of about  $k_B \cdot 10 \mu\text{K}$ , which may be in reach with current Paul traps and state-of-the-art excess micromotion compensation.

In the article [H6], in collaboration with the group of Prof. Rene Gerritsma at the University of Amsterdam, we investigated cold collisions between  $\text{Yb}^+$  ions and  $^6\text{Li}$  atoms. Rates for chemical reactions between  $^6\text{Li}$  atoms and  $^{171}\text{Yb}^+$ ,  $^{174}\text{Yb}^+$  and  $^{176}\text{Yb}^+$  ions in the mK regime were experimentally determined. We showed that the reaction rate for atoms and ions in the electronic ground state is at least  $10^3$  times smaller than the Langevin collision rate, which should be sufficiently small for sympathetic cooling and quantum applications.

These findings were in agreement with recent calculations [O4][166]. Furthermore, the ions were prepared in excited electronic states and it was shown that the main reaction process occurring in this situation is charge transfer. We found that for the  $^2P_{1/2}$  and  $^2F_{7/2}$  state in  $^{174}\text{Yb}^+$  and  $^{176}\text{Yb}^+$ , the charge transfer rate approaches the Langevin collision rate, whereas for the metastable  $^2D_{3/2}$  state, we found rates that are more than an order of magnitude smaller. We showed that the charge transfer rate is almost independent of the collision energy, suggesting that charge transfer is associated with Langevin collisions. Our results did not depend strongly on the ionic isotope. The low charge transfer rate for ground state collisions were corroborated by theory, but the  $4f$  shell in the  $\text{Yb}^+$  ion prevented an accurate prediction for the charge transfer rate of the  $^2P_{1/2}$ ,  $^2D_{3/2}$  and  $^2F_{7/2}$  states. Using *ab initio* methods of quantum chemistry we calculated the ion-atom interaction potentials up to energies of  $30 \times 10^3 \text{ cm}^{-1}$  (see Fig. 6), and used these to give qualitative explanations of the observed rates.

For ion-atom mixtures to be used in quantum technology applications – in which quantum information will be stored in the internal states of the ions and atoms – it is required that spin-changing collision rates are small [167]. In a recent experiment very fast spin dynamics in  $\text{Yb}^+$  ions interacting with Rb atoms was shown [168]. Besides fast spin exchange – which conserves the total spin of the collision partners – strong spin-nonconserving rates known as spin-relaxation were also observed.

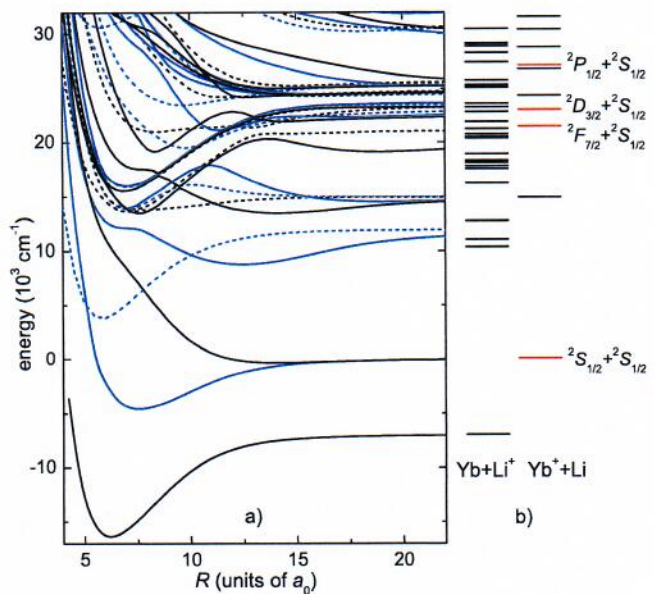


Figure 6: Energy spectrum of the  $(\text{Yb}+\text{Li})^+$  system: a) Nonrelativistic potential energy curves of the  $\text{LiYb}^+$  molecular ion. Black and blue lines correspond to singlet ( $S = 0$ ) and triplet ( $S = 1$ ) states, whereas solid and dashed lines represent states with the projection of the electronic orbital angular momentum on the molecular axis equal to zero ( $\Lambda = 0$ ,  $\Sigma$  symmetry) and non-zero ( $|\Lambda| > 0$ ), respectively. The lowest 5 electronic states are taken from Ref. [O5]. b) Possible ion-atom dissociation thresholds with thresholds investigated in this work highlighted in red. Experimental energies are taken from the NIST database [165]. From the article [H6].

Theoretical calculations suggested that an exceptionally large second-order spin-orbit coupling in  $\text{Yb}^+/\text{Rb}$  provided a mechanism for the observed spin-relaxation rates [169]. For  $\text{Yb}^+/\text{Li}$  the second-order spin-orbit coupling was expected to be much smaller.

In the article [H5], in continued collaboration with the group of Prof. Rene Gerritsma at the University of Amsterdam, we investigated the spin dynamics of single trapped  $\text{Yb}^+$  ions in a cold, spin-polarized bath of  $^6\text{Li}$  atoms. Specific (pseudo-) spin states in the ion were prepared by optical pumping and microwave pulses. Electron shelving and fluorescence detection allowed to determine the spin state after interacting with the atomic cloud. For  $^{174}\text{Yb}^+$  we found that the cloud of atoms polarizes the spin of the ion by 93(4)%. Our results indicated a very large spin-exchange rate of  $1.03(12) \cdot \gamma_L$ , whereas spin-relaxation rates were estimated to be  $\leq 0.08(4) \cdot \gamma_L$ . Here,  $\gamma_L = 2\pi\rho_{\text{Li}}\sqrt{C_4/\mu} = 22(7) \text{ s}^{-1}$  is the Langevin collision rate, with  $\rho_{\text{Li}}$  the density of Li atoms at the location of the ion,  $C_4$  is proportional to the polarizability of the atom and  $\mu$  is the reduced mass. For the  $^{171}\text{Yb}^+$  isotope, all four hyperfine ground states were prepared and all decay rates were measured. As in  $^{174}\text{Yb}^+$ , we found strong rates towards spin polarization. However, relaxation from the  $m_F = 1$  state towards the  $F = 0$  ground state occurred at a rate of  $0.13(3) \cdot \gamma_L$ . We combined *ab initio* quantum scattering calculations with the measured spin dynamics (see Fig. 7). Interestingly, we found in our calculations that even in the mK temperature regime the spin-exchange rates still depend strongly on the difference between assumed singlet ( $a_S$ ) and triplet ( $a_T$ ) scattering lengths. Our results indicated a large difference between the singlet and triplet scattering lengths in  $\text{Yb}^+/\text{Li}$ , which would be beneficial for the observation of Feshbach resonances. Our electronic structure calculations also confirmed that spin-nonconserving relaxation rates due to second-order spin-orbit coupling should be smaller than for  $\text{Yb}^+/\text{Rb}$ .

My collaboration with the group of Prof. Rene Gerritsma at the University of Amsterdam continues and recently we have obtained groundbreaking results on sympathetic cooling to the quantum regime of ion-atom collisions in the  $\text{Yb}^+-\text{Li}$  system, which will be published soon.

### Cold interactions and chemical reactions of linear polyatomic anions with metal atoms

After many spectacular successes in the field of ultracold atoms, the scientific community has drawn its attention to the research on ultracold molecules. Recently, ultracold gases of diatomic molecules have been produced and explored. The next emerging goal is the preparation of polyatomic molecules at ultralow temperatures and the first experiments have been launched. Molecular ions are easier to prepare, trap, and detect as compared to neutral molecules. They are also important in many areas of chemistry ranging from organic and inorganic chemistry to astrochemistry. Therefore polyatomic molecular ions are promising systems to start investigating cold polyatomic dynamics and chemical reactions at the quantum level. Recently, first experiments combining simple diatomic molecular ions with ultracold atoms have been launched. The dynamics of  $\text{N}_2^+$  molecular cations immersed in ultracold Rb atoms [170] and  $\text{BaCl}^+$  cations immersed in ultra-

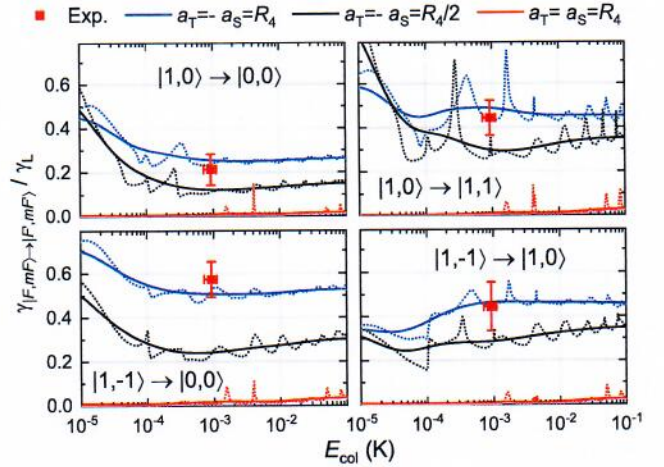


Figure 7: Spin-exchange transition rates for  $^{171}\text{Yb}^+$  versus collision energy obtained in coupled-channel scattering calculations for three sets of scattering lengths compared with measured rates (red squares). Dotted lines are energy-resolved rates and solid lines are thermally averaged rates. From the article [H5].

cold Ca atoms [73, 75] was investigated. The collisions of  $\text{OH}^-$  molecular anions with ultracold Rb atoms were studied both experimentally [171, 172] and theoretically [172–176]. The cooling of simple molecular ions such as  $\text{MgH}^+$ ,  $\text{NH}_2^-$ , and  $\text{OH}^-$  immersed in cold buffer gases of helium or molecular hydrogen were also experimentally [74, 177–181] and theoretically [182–184] investigated.

In the article [H7], I considered collisional studies of linear polyatomic ions immersed in ultracold atomic gases and investigated the intermolecular interactions and chemical reactions of several molecular anions ( $\text{OH}^-$ ,  $\text{CN}^-$ ,  $\text{NCO}^-$ ,  $\text{C}_2\text{H}^-$ ,  $\text{C}_4\text{H}^-$ ) with alkali-metal (Li, Na, K, Rb, Cs) and alkaline-earth-metal (Mg, Ca, Sr, Ba) atoms. Selected diatomic molecular anions are important in many areas of chemistry, whereas considered polyatomic molecular anions are of great interest to astrochemistry [185]. I applied state-of-the-art *ab initio* techniques to compute the potential energy surfaces (PESs) for these systems. The coupled cluster method restricted to single, double, and noniterative triple excitations, CCSD(T), was employed and the scalar relativistic effects in heavier metal atoms were modeled within the small-core energy-consistent pseudopotentials. The leading long-range isotropic and anisotropic induction and dispersion interaction coefficients were obtained within the perturbation theory. The PESs were characterized in detail and their universal similarities typical for systems dominated by the induction interaction were discussed. The two-dimensional PESs were provided for selected systems and can be employed in scattering calculations. The possible channels of chemical reactions and their control were analyzed based on the energetics of reactants. I showed that most of the considered anion-atom systems are stable against chemical reactions and charge transfer processes which however can be induced by exciting atoms or anions with the laser field. Thus the presented work paved the ways for collisional studies and sympathetic cooling of linear polyatomic ions immersed in ultracold atomic gases and their applications in controlled chemistry, precision measurements, and quantum simulation.

### Rotation of cold molecular ions inside a Bose-Einstein condensate

Cold molecular ions are a versatile platform to study single-, few-, and many-particle quantum processes [78, 186, 187]. As opposed to neutral molecules [187], the degree of freedom used to manipulate molecular ions – their charge – is effectively decoupled from their internal structure, and therefore even complex species can be trapped and cooled down to milliKelvin translational temperatures [186]. Molecular ions can be prepared in a selected rovibrational state by optical pumping [188] or sympathetic cooling of state-selected ions [189]. They can also be trapped for a few hours, with the rotational state lifetimes exceeding 15 minutes [189]. Recently, rotational motion of molecules immersed in a Bose-Einstein condensate was described by quasiparticles of a new kind – the ‘angulons’ [190, 191]. In this model rotating molecules are dressed by a field of many-body excitations. In this way, angulons are a rotational analogue of polarons [192, 193], actively studied experimentally in ultracold quantum gases [105, 194–203]. However, the non-Abelian algebra and discrete energy spectrum associated with quantum rotations makes the angulon physics drastically different compared to any polaron problem, where the translational motion of an impurity is studied.

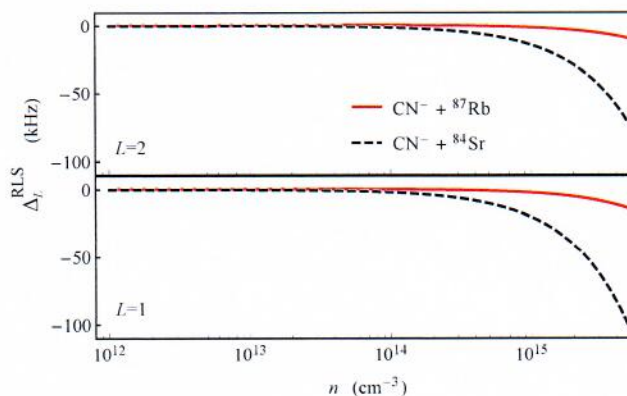


Figure 8: Differential rotational Lamb shifts for  $\text{CN}^- + ^{87}\text{Rb}$  (red solid curve) and  $\text{CN}^- + ^{84}\text{Sr}$  (black dashed curve), as a function of the BEC density,  $n$ , on a logarithmic scale. From the article [H8].

Table 1: The hybrid heteronuclear ion-atom systems without charge transfer radiative losses among the combinations of the present experimentally accessible laser-cooled trapped ions and ultracold atoms.

Nature of ion/atom	Systems without charge transfer radiative losses
open-shell/open-shell	$Ba^+/Li$ , $Ca^+/Cr$ , $Sr^+/Cr$ , $Ba^+/Cr$ , $Yb^+/Cr$ , $Sr^+/Dy$ , $Ba^+/Dy$ , $Sr^+/Er$ , $Ba^+/Er$
open-shell/closed-shell	$Ca^+/Mg$ , $Sr^+/Mg$ , $Ba^+/Mg$ , $Yb^+/Mg$ , $Sr^+/Ca$ , $Ba^+/Ca$ , $Ba^+/Sr$ , $Ca^+/Yb$ , $Sr^+/Yb$ , $Ba^+/Yb$
closed-shell/open-shell	$Na^+/Li$ , $K^+/Li$ , $Rb^+/Li$ , $Cs^+/Li$ , $K^+/Na$ , $Rb^+/Na$ , $Cs^+/Na$ , $Rb^+/K$ , $Cs^+/K$ , $Cs^+/Rb$ alkali-metal ion/ $Cr$ , alkali-metal ion/ $Dy$ , alkali-metal ion/ $Er$
closed-shell/closed-shell	alkali-metal ion/alkaline-earth-metal atom (except $Li^+/Ba$ )

In the article [H8], in collaboration with the group of Prof. Mikhail Lemeshko at the Institute of Science and Technology in Vienna, we used recently developed angulon theory [190, 191] to study the rotational spectrum of a molecular ion immersed into a Bose-Einstein condensate. As a concrete experimental system we considered a single cyanide ( $CN^-$ ) anion immersed into an atomic BEC of  $^{87}Rb$  and  $^{84}Sr$ . We exemplified our technique with molecular anions, since those have been used in the context of hybrid ion-atom setups in order to achieve sympathetic cooling [171]. Furthermore, negative ions have been used to study cold rotationally inelastic [172, 176, 179] and reactive [177] collisions, and are highly relevant for astrochemistry [204]. It is worth noting, however, that the predicted effects are not expected to change substantially, either qualitatively or quantitatively, for the case of positive molecular ions. Based on *ab initio* potential energy surfaces, we provided a detailed study of the rotational Lamb shift and many-body-induced fine structure which arise due to dressing of molecular rotation by a field of phonon excitations. We demonstrated that the magnitude of these effects is large enough in order to be observed in modern experiments on cold molecular ions. In particular, the rotational Lamb shifts were evaluated to be on the order of a few kHz (see Fig. 8). Furthermore, we introduced a novel method to construct pseudopotentials starting from the *ab initio* potential energy surfaces, which provides a means to obtain effective coupling constants for low-energy polaron models.

### Ultracold magnetically tunable interactions without radiative charge transfer losses between $Ca^+$ , $Sr^+$ , $Ba^+$ , and $Yb^+$ ions and $Cr$ atoms

In hybrid systems of laser-cooled trapped ions and ultracold atoms combined in a single experimental setup, losses due to radiative inelastic processes, that is the radiative charge transfer and radiative association [68, 167], are the basis of controlled ion-atom chemistry [79] but they can obstruct sympathetic cooling [67], and interesting applications in quantum computing [72] and quantum simulation of many-body physics [71]. Radiative losses can be reduced by choosing a system with a favorable electronic structure such as  $Yb^+ + Li$  [O4] and avoided if, and only if, an interacting ion-atom system is in its absolute electronic ground state and the charge transfer is impossible. This condition is met when the ionization potential of an atom is larger than the electron affinity of a positive ion. Up to date, all experimentally investigated cold heteronuclear hybrid ion-atom systems have presented radiative losses [66–69, 168, 205–212]. These losses are unavoidable for almost all alkaline-earth-metal and ytterbium ions immersed in a cold gas of alkali-metal atoms [89, 166, 213–216] (except the  $Ba^+$  ion in a gas of the  $Li$  atoms). They can be, however, avoided for some combinations of alkali-metal ions interacting with alkali-metal atoms [217] or alkaline-earth-metal ions interacting with alkaline-earth-metal atoms [210] and for almost all combinations of alkali-metal ions interacting with alkaline-earth-metal atoms (except the  $Li^+$  ion in a gas of the  $Ba$  atoms) [cf. Table 1]. Homonuclear ion-atom systems do not suffer from radiative losses but show resonant spin-changing charge-exchange inelas-

tic collisions [218–220]. Unfortunately, the preparation and manipulation of laser-cooled closed-shell alkali-metal ions and closed-shell alkaline-earth-metal atoms are experimentally more challenging than using open-shell ones. Furthermore, the magnetically tunable Feshbach resonances predicted for mixtures of closed-shell and open-shell species are very narrow [221, 222]. Therefore, the useful control of ultracold ion-atom interactions with magnetically tunable Feshbach resonances should be expected only when both ions and atoms are of the open-shell nature [100].

In the article [H9], I proposed the  $\text{Ca}^+$ ,  $\text{Sr}^+$ ,  $\text{Ba}^+$ , and  $\text{Yb}^+$  ions immersed in an ultracold gas of the Cr atoms as experimentally feasible heteronuclear systems in which ion-atom interactions at ultralow temperatures can be controlled with magnetically tunable Feshbach resonances without charge transfer and radiative losses. Among the present experimentally accessible laser-cooled trapped ions and ultracold atoms, the other possible combinations are the  $\text{Ba}^+$  ions and the Li atoms as well as the  $\text{Sr}^+$  or  $\text{Ba}^+$  ions and the Dy or Er atoms. I applied *ab initio* techniques to investigate electronic-ground-state properties of the  $\text{CaCr}^+$ ,  $\text{SrCr}^+$ ,  $\text{BaCr}^+$ , and  $\text{YbCr}^+$  molecular ions. The interaction of the  $^2S$  state alkaline-earth-metal or ytterbium ion with the  $^7S$  state chromium atom gives rise to the two molecular electronic states of the  $X^6\Sigma^+$  and  $a^8\Sigma^+$  symmetries [223]. The potential energy curves, permanent electric dipole moments, and static electric dipole polarizabilities were computed. The spin restricted open-shell coupled cluster method restricted to single, double, and noniterative triple excitations, RCCSD(T), and the multireference configuration interaction method restricted to single and double excitations, MRCISD, were employed. The scalar relativistic effects were included within the small-core energy-consistent pseudopotentials. The leading long-range induction and dispersion interaction coefficients were also reported. Finally, magnetic Feshbach resonances between the  $\text{Ca}^+$ ,  $\text{Sr}^+$ ,  $\text{Ba}^+$ , and  $\text{Yb}^+$  ions interacting with the Cr atoms were analyzed. The presented proposal paved the way towards more elaborate studies of the formation and application of hybrid ion-atom systems free of radiative charge transfer losses.

### Ultracold isotope-exchange reactions between heteronuclear dimers in external fields

Ultracold molecules have recently become a new powerful tool for investigating chemistry at its fundamental quantum limit [12]. The production of an ultracold high phase-space-density gas of polar molecules in their absolute rovibrational ground state [23–25] allowed for groundbreaking experiments on controlled chemical reactions [29–31]. An unprecedented control over the quantum states of reactants both by selecting their internal states and by tuning dipolar collisions with an external electric field in a reduced dimensionality were achieved. The next expected milestone towards the state-to-state ultracold controlled chemistry will be the measurement and control of the product-state distributions [224].

The quantum statistics [29], quantum tunneling and reflection from a centrifugal barrier [225], as well as the impact of external fields [31] can modify the rates for ultracold chemical reactions by many orders of magnitude because at ultralow temperatures the reactants can be prepared in a single quantum state and even a weak perturbation can be comparable to or larger than the collision energy [224]. At the same time, the energy released in a chemical reaction between  $^1\Sigma^+$ -state polar alkali-metal molecules in the ground rovibrational level, if energetically allowed, is at least 12 K for K<sub>2</sub>, or more for other molecules [226]. This means that untrappable products in many states with relatively large kinetic energy are expected and thus prospects for observing quantum effects and control in product distributions are limited [227]. For this reason, the rate constants for ultracold reactive collisions of the K<sub>2</sub> molecules were shown to be universal, that is, independent of the short-range dynamics [225].



In the article [H10], I proposed ultracold isotope-exchange reactions between heteronuclear dimers—a prototype of atom-exchange reactions—as a promising system for investigating models of the controlled chemical reactivity. I showed that isotope-exchange reactions between ground-state alkali-metal, alkaline-earth-metal, and lanthanide heteronuclear dimers consisting of two isotopes of the same atom are exothermic with an energy change in the range of 1-8000 MHz thus resulting in cold or ultracold products. For these chemical reactions there are only one rovibrational and at most several hyperfine possible product states with the kinetic energy in the cold or ultracold regime. The number and energetics of open and closed reactive channels can be controlled by the laser and magnetic fields. I demonstrated that these exothermic chemical reactions can be tuned to become endothermic by employing light near-resonant with a molecular bound-to-bound transition in the heteronuclear reactant while off-resonant for homonuclear products, that is, isotope- and state-selective AC Stark shift control (cf. Fig. 9). Application of the magnetic field can bring an additional control over the number and energetics of open and closed reactive channels. The proposed systems and required field strengths are all within the current experimental capabilities. The demonstrated control schemes are also applicable to other isotope-exchange reactions e.g. in ultracold mixtures of molecules and atoms. The presented proposal paved the way for studying the state-to-state dynamics of ultracold chemical reactions beyond the universal limit with a meaningful control over the quantum states of not only reactants but also products.

#### 4. Summary

Summing up, the realization of the projects constituting the presented scientific achievement significantly increased the knowledge about properties, interactions, cold collisions, chemical reactions, and controllability with external fields of ultracold quantum mixtures of atoms, ions, and molecules – the systems, which are interesting from the fundamental point of view. We proposed and investigated new concepts, systems, and tools. We paved the way for new developments and studies on ultracold quantum matter and new ways of engineering ultracold controllable atomic, ionic, and molecular systems and their applications in studying various quantum phenomena. The obtained theoretical results explained, guided and inspired ongoing and upcoming experimental works. In the end, all anticipated efforts are bringing a better understanding of the quantum nature of the world at the microscopic level, essential for all branches of physics and natural sciences.

At the moment, together with my research group and in close collaboration with experimental partners, I continue intensive studies of cold interactions and collisions in atomic, ionic, and molecular systems, and their applications ranging from precision measurements to quantum simulation.

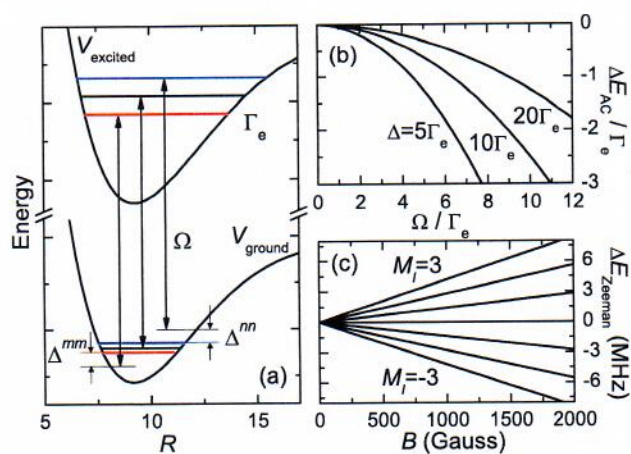


Figure 9: (a) Scheme of the state-selective AC Stark shift control. Different levels corresponds to different isotope mixtures (energies are not in scale). (b) The AC Stark shift for different laser detunings vs. the laser field Rabi frequency  $\Omega$ . (c) Zeeman levels of  $^{87}\text{Rb}_2$  vs. the magnetic field. From the article [H10].

Tamara

## V. OTHER RESEARCH ACCOMPLISHMENTS

### A. BIBLIOMETRIC DATA (24.04.2019)

- number of published and accepted articles: **24**
- total number of citations without self-citations: **256** (acc. Web of Science)
- h-index (Hirsch index): **12** (acc. Web of Science)
- sum of impact factors: **126,1**
- research grants: **4** (2 from NCN, 2 from FNP) - **4,3 mln** PLN in total
- supervision: **4** B.Sc. students, **3** M.Sc. students, **4** Ph.D. students (ongoing), **2** postdocs
- invited talks at international conferences: **4**
- contributed talks at international conferences: **18**
- invited seminars abroad: **14**
- invited seminars in Poland: **11**
- reviewed articles for international journals: **32**
- reviewed Ph.D. theses abroad: **2**

*Detailed information is collected in Załącznik nr 4 (Appendix 4).*

### B. LIST OF PUBLICATIONS NOT INCLUDED IN THE ACHIEVEMENT INDICATED IN PT. IV

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### C. DESCRIPTION OF RESEARCH NOT INCLUDED IN THE ACHIEVEMENT INDICATED IN PT. IV

I have started my research work in the field of quantum chemistry and theoretical atomic, molecular and optical physics in 2008, while preparing my M.Sc. thesis on "Two-photon photoassociation of cold atoms in a femtosecond laser field", which was defended with a distinction in 2009 and distinguished by the Prof. Rychlewski Award of the Polish Chemical Society for the best thesis in quantum chemistry in Poland. In my M.Sc. thesis I investigated coherent control of two-photon photoassociation of ultracold Ca atoms in the field of femtosecond laser pulses using effective two-state Hamiltonian in the rotating wave approximation. I calculated potential energy curves, two-photon transition dipole moments, and dynamic polarizabilities using response theory formulated within the coupled cluster method. The Chebyshev propagator was used to solve the time-dependent Schrödinger equation. Laser pulses were shaped both in the frequency domain in the weak-field regime and in the time domain in the strong-field regime. The goal of this project was to find conditions for efficient two-photon photoassociation of ultracold atoms into ultracold molecules, when atomic excitation is coherently suppressed while the formation of weakly-bound molecules red-detuned with respect to the atomic threshold is enhanced. The thesis was realized at the University of Warsaw under the supervision of prof. dr. hab. Robert Moszyński and in collaboration with prof. dr. Christiane Koch.

Next, I used the computational scheme established in my M.Sc. thesis in calculations for a large theoretical and experimental collaboration which goal was to show femtosecond coherent control of two-photon photoassociation of thermal Mg atoms into Mg<sub>2</sub> molecules. For this project, I calculated potential energy curves, two-photon transition dipole moments, and dynamic polarizabilities. Experiments were conducting by the group of Prof. Zohar Amitay at Technion - Israel Institute of Technology and the results of this collaboration were presented in publications [O12], [O11], [O8]. The most important finding was the demonstration of the formation of diatomic molecules with rotational and vibrational coherence in free-to-bound two-photon femtosecond photoassociation of hot atoms. The coherent superpositions of bound rovibrational levels in an electronically excited state were probed by a time-delayed third photon and generation of coherence was explained by Franck-Condon filtering of collision energies and partial waves. Those results paved the way to coherent control of bond making [228].

My graduate studies started in 2009 and concerned theoretical investigations of the quantum dynamics and control of ultracold molecules in external fields. My Ph.D. thesis on "Quantum dynamics and control of ultracold molecules in external fields" was defended in 2014 under the supervision of prof. dr. hab. Robert Moszyński at the University of Warsaw and prof. dr. Christiane Koch at the University of Kassel in Germany. The new schemes of the formation and quantum control were proposed and investigated and paved the way towards the ultimate goal of the full quantum control over molecular processes. The state-of-the-art *ab initio* methods were applied to investigate the electronic structure of molecular systems important for the ongoing or planned experimental and theoretical research at ultralow temperatures. Next, the electronic structure data were employed in both time-dependent and time-independent studies of molecular dynamics in the number of projects on the structure, formation, control, and collisions of ultracold atoms and molecules. Six publications [O13], [O10], [O9], [O7], [O6], and [O5] constituted the core of the thesis. All programs written as a part of the graduate research were included in the library of programs for the simulation of time-dependent quantum molecular dynamics QDYN developed in the group of prof. dr. Christiane Koch at the University of Kassel in Germany.

In the article [O14], we investigated the electronic structure of the SrYb molecule for the first time and employed it to investigate the possibility of forming deeply bound ultracold SrYb molecules in an optical lattice in a photoassociation experiment using continuous-wave lasers, the first reported in the literature investigation of the formation of a polar ultracold molecule from two closed-shell atoms. Photoassociation near the intercombination line transition of atomic strontium into the vibrational levels of the strongly spin-orbit mixed  $b^3\Sigma^+$ ,  $a^3\Pi$ ,  $A^1\Pi$ , and  $C^1\Pi$  states with subsequent efficient stabilization into the  $v'' = 1$  vibrational level of the electronic ground state was proposed. Ground state SrYb molecules can be accumulated by making use of collisional decay from  $v'' = 1$  to  $v''' = 0$ . Alternatively, photoassociation and stabilization to  $v'' = 0$  can proceed via stimulated Raman adiabatic passage provided that the trapping frequency of the optical lattice is large enough and phase coherence between the pulses can be maintained over at least tens of microseconds.

In the article [O10], in collaboration with Prof. Monika Musiał at the University of Silesia in Katowice, we investigated the electronic structure of the Rb<sub>2</sub> molecule by employing the double electron attachment intermediate Hamiltonian Fock space coupled cluster method restricted to single and double excitations for all electronic states up to and including the  $5s + 5d$  dissociation limit at about  $26,000 \text{ cm}^{-1}$ . The calculation was the first reported in literature use of this recently developed method to generate highly accurate interatomic interaction potentials. In order to correctly predict the spectroscopic behaviour of Rb<sub>2</sub>, the electric transition dipole moments, non-adiabatic coupling and spin-orbit coupling matrix elements, and static dipole polarisabilities were also calculated with the multireference configuration interaction method. The influence of the non-resonant laser light on the rovibrational structure of open-shell molecules was also investigated. The spectroscopic sig-

natures of this effect in  $\text{Rb}_2$  molecule for transitions between the  $X^1\Sigma_g^+$  electronic ground state and the  $A^1\Sigma_u^+$  and  $b^3\Pi_u$  excited state manifold were studied. The latter is characterized by strong perturbations due to the spin-orbit interaction. For non-resonant field strengths of the order  $10^9 \text{ W/cm}^2$ , the spin-orbit interaction and coupling to the non-resonant field become comparable. Thus, the non-resonant field can then be used to control the singlet-triplet character of rovibrational levels.

In the article [O8], I proposed and investigated a new class of highly magnetic and polar molecules consisting of chromium and closed-shell alkali-metal atoms. These molecules are examples of species possessing large both magnetic and electric dipole moments making them potentially interesting candidates for ultracold many-body physics studies. Especially, the competition between the magnetic and electric dipolar interactions and the control with external electric and magnetic fields can be realized and investigated with these molecules .

In the article [O7], in collaboration with Prof. Roman Krems at the University of British Columbia in Vancouver, we investigated the interactions of polar alkali-metal dimers in the quintet spin state and we demonstrated the formation of deeply bound reaction complexes. The reaction complexes can decompose adiabatically into homonuclear alkali-metal dimers (for all molecules except  $\text{KRb}$ ) and into alkali-metal trimers (for all molecules) with no barriers for these chemical reactions. This means that all alkali-metal dimers in the  $a^3\Sigma^+$  state are chemically unstable at ultracold temperatures, and the use of an optical lattice to segregate the molecules and suppress the losses may be necessary. The unique features of the chemical reactions of ultracold alkali-metal dimers in the  $a^3\Sigma^+$  electronic state that can be control with external electric fields were discussed.

In the article [O6], we proposed the non-resonant laser light to be used to engineer the Feshbach resonances in their position and width in polar paramagnetic ground-state molecules. Magnetically tunable Feshbach resonances in such molecules are too narrow to allow for magnetoassociation starting from trapped, ultracold atoms. For non-resonant field intensities of the order of  $10^9 \text{ W/cm}^2$ , we found the width to be increased by three orders of magnitude, reaching a few Gauss. This paved the way for producing ultracold molecules with sizeable electric and magnetic dipole moments and thus for many-body quantum simulations with such particles.

In the article [O5], I proposed and investigated the properties of the electronic ground state of the polar and paramagnetic europium-*S*-state-atom molecules. *Ab initio* techniques were applied to compute the potential energy curves for the europium-alkali-metal-atom, europium-alkaline-earth-metal-atom, and europium-ytterbium molecules in the Born-Oppenheimer approximation for the high-spin electronic ground state. The  $\text{EuK}$ ,  $\text{EuRb}$ , and  $\text{EuCs}$  molecules were found as examples of species possessing both large electric and magnetic dipole moments making them potentially interesting candidates for ultracold many-body quantum simulation when confined in an optical lattice in combined electric and magnetic fields.

In the article [O4], we investigated the electronic structure of the  $\text{LiYb}^+$  molecular ion for the first time and the results of *ab initio* calculations were employed in the scattering calculations. The prospects for the sympathetic cooling of the  $\text{Yb}^+$  ion emerged into ultracold gas of Li atoms were investigated. The rates for the elastic and inelastic due to the radiative charge transfer and radiative association collisions were calculated. The photoassociation spectra for the one-photon formation of the singlet state molecular ion and for the two-photon formation of the triplet state molecular ion were evaluated and single molecule photoassociation spectroscopy was proposed. Consequences of the present results for building a quantum simulator emulating solid-state physics with a hybrid system of ultracold Yb ions and Li atoms were analyzed.

During my postdoctoral stay at the Institute of Photonic Science in Barcelona, I focused part of my research interests on problems of quantum many-body systems. In the articles [O2] and [O3], in collaboration with Prof. Maciej Lewenstein, we employed *ab initio* methods of quantum chemistry to investigate spin-1/2 fermions interacting via a two-body contact potential in a one-dimensional

harmonic trap. We also studied the crossover between few and many fermions in a harmonic trap, where we found that the energy converges surprisingly rapidly to the many-body result for every value of the interaction strength, whereas many more particles are needed to give rise to the non-analytic behavior of the pairing gap, and to smoothen the pronounced even-odd oscillations of the chemical potential induced by the shell structure of the trap. I continue this line of research with part of my research group investigating few- and many-body systems of highly-magnetic and polar molecules and polar molecular ions.

After returning back to the University of Warsaw at the end of 2016, I established my research group to actively realize my numerous scientific ideas and projects. I have enrolled several B.Sc. and M.Sc. students, four Ph.D. students, and one postdoctoral researcher. We aim to work at the forefront of atomic, molecular, and optical physics and quantum chemistry, in close collaboration with my international theoretical and experimental research partners, selecting systems, problems, and applications that are the most relevant for ongoing and upcoming experimental works.

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