

Charge and spin collisional dynamics in cold ion-atom systems

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Hybrid systems of laser-cooled trapped ions and ultracold atoms combined in a single experimental setup have recently emerged as a new platform for fundamental research in quantum physics and chemistry [1]. Reaching ultracold s-wave quantum regime is one of the most important challenges in this field at the moment. Unfortunately, the lowest attainable temperatures in experiments using the Paul ion trap are limited by the rf-field-induced heating related to the micromotion [2]. A possible solution to this problem is the use of ion-atom mixtures with the large ion-to-atom mass ratio [2]. The Yb^+/Li combination is the best candidate among mixtures which allows for straightforward laser cooling of both ions and atoms.

I will present how *ab initio* quantum chemistry calculations support and guide quantum physics experiments in our experimental-theoretical collaboration with the group of Prof. Rene Gerritsma at the University of Amsterdam. The radiative charger transfer and association losses theoretically predicted for the Yb^+/Li system to be small [3] were recently experimentally confirmed [4] opening the way for sympathetic cooling and application in quantum simulation [5]. Additionally, we showed and explained that the charge transfer rate constants for ions in excited electronic states are three orders of magnitude larger [4]. Next, we investigated the spin dynamics of single trapped Yb^+ ions in a cold, spin-polarized bath of ^6Li atoms [6]. We combined *ab initio* quantum scattering calculations with the measured spin dynamics and found that even in the mK temperature regime the spin-exchange rate constants still depend strongly on the difference between assumed singlet and triplet scattering lengths. Our results indicated a large difference between the singlet and triplet scattering lengths in $\text{Yb}^+/^6\text{Li}$, which would be beneficial for the observation of Feshbach resonances [6]. Finally, the first results towards reaching quantum regime of ion-atom collisions and observing collision resonances have recently been obtained.

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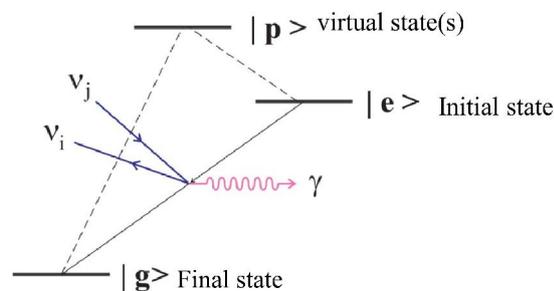
Radiative emission of neutrino pair from atoms and molecules: theoretical estimation of emission spectra

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Neutrinos are the most common particles, next to 3K photons, in the present universe, however some of their properties, including their absolute masses and mass type (Majorana or Dirac), have not yet determined experimentally, because these neutrinos are neutral and interact with the other particles only through the weak interaction. Although the conventional target for exploration of neutrino properties has been nuclei, it has recently been discussed that atoms and molecules may become good targets for determining neutrino parameters such as the neutrino mass type (Majorana or Dirac), and the CP violating phases including Majorana phases [1-3]. Most of these observables are difficult to measure in neutrino oscillation experiments. In this work, we consider deexcitation of atoms or molecules in a metastable level $|e\rangle$ emitting a neutrino pair and a photon; $|e\rangle \rightarrow |g\rangle + \gamma + \nu_i \nu_j$ where ν_i 's are neutrino mass eigenstates. This process exists as a combined effect of second order in the electromagnetic interaction and the weak interaction of the standard electroweak theory, as schematically shown in the figure below. The shape of photon spectra from this process reflect the properties of neutrinos, namely unknown neutrino parameters. In this work, we compute the photon spectra arising from the radiative neutrino pair emission processes of metastable excited states of I_2 molecule [4] and Au atom, and will discuss how the spectra shape depend on the neutrino parameters [5].



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Visualization technique of dynamical reaction pathways: application to non-IRC pathways of SN2 reaction

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[Introduction] The intrinsic reaction coordinate (IRC) is defined as a minimum energy pathway connecting two minimum structures (MINs) *via* a transition state structure (TS) on the potential energy surface (PES) and gives an intuitive picture of chemical reaction. Recently, the global reaction route mapping (GRRM) strategy has been proposed, which enables us to construct a global reaction route network by exploring the IRC pathways systematically.¹ The global reaction route network for a given molecular system is a useful tool to predict unknown chemical reactions, but there was no attempt to visualize the network to 2- or 3- dimensional coordinate space. Very recently, we employed a classical multidimensional scaling (MDS) method to embed multidimensional data into the lower-dimensional space with preserving their mutual distances as much as possible. The results revealed that classical MDS finds significant principal coordinates which describe structural transformations well without background knowledge.²

In the reaction dynamics fields, *ab initio* molecular dynamics (AIMD) method without potential functions has been carried out. By following the structural changes along the AIMD trajectories, the dynamical reaction processes can be obtained, but it is not an easy task to grasp an intuitive picture from complicated massive time-series data. In this study, we project the dynamical reaction pathways of AIMD trajectories into 2-dimensional principal coordinate space determined by classical MDS to elucidate the dynamics effects on reaction path picture. The target is the SN2 reaction of $\text{OH}^- + \text{CH}_3\text{F} \rightarrow [\text{CH}_3\text{OH}\dots\text{F}]^-$ for which the previous study shows that 90% of AIMD trajectories starting from TS did not follow the IRC pathway.³ By applying classical MDS to the single IRC pathway, AIMD trajectories are projected into the reaction route map spanned by the 2-dimensional principal coordinates.

[Computational details and results] We calculated the IRC pathway at MP2/6-31+G* level and carried our AIMD simulations with 50 trajectories from TS to the product region at the same computational level. **Fig. 1** shows that 101 structures along the IRC pathway are embedded in 2-dimensional principal coordinate space. By mapping 50 trajectories into this 2-dimensional coordinate space, we can show that 43 trajectories are assigned as direct dissociation pathways, which deviate from the IRC pathway at a large curvature region due to dynamics effects. In this presentation, the details of methodologies and dynamical reaction pathways of trajectories will be presented.

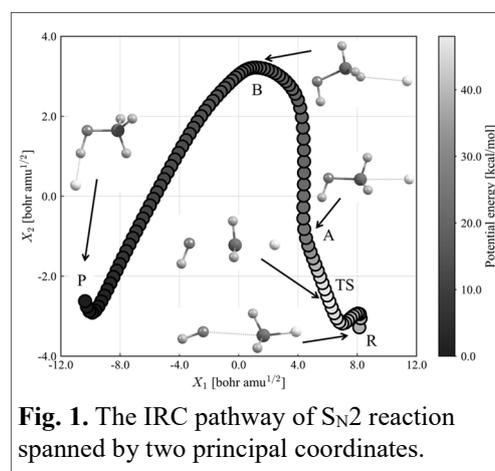


Fig. 1. The IRC pathway of SN2 reaction spanned by two principal coordinates.

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Generation of Anharmonic Potential Energy Surface Using SINDO

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We have developed a suite of programs, SINDO, which generates the potential energy surface (PES) of polyatomic molecules based on normal coordinates and solves the vibrational Schrödinger equation with the PES. In this presentation, I will introduce latest updates in the PES generator of SINDO, which has the following features:

1. Generation of a quartic force field (QFF). [1]
2. Generation of a grid PES based on harmonic oscillator DVR. [2]
3. A combination of QFF and grid PES based on a multiresolution method. [3]
4. A comprehensive, streamlined input based on Extensible Markup Language (XML).
5. A portable interface with GAUSSIAN and other *ab initio* programs to obtain the energy and gradients.
6. Parallel calculations over grid points.

I will show recent applications to vibrational calculations of a protonated water tetramer, $\text{H}^+(\text{H}_2\text{O})_4$ [4], and a solute/solvent system and biomolecules based on a PES derived from the QM/MM calculations [5].

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