QSS06 - Kang-Kuen Ni - Questions & Answers

Kang-Kuen Ni

Yutaka Shikano: How to understand the reaction rate in the ultracold chemistry? Is this the energy landscape viewpoint still valid to understand the reaction rate?

KANG-KUEN: In an ultracold reaction, the reaction rate is usually about the "collision rate" (in many cases, it is equal to the collision rate), which is determined by the long-range forces that bring the reactants together. The energy landscape shows the long-range potential and can be used to determine how fast pairs of molecules are found in the "short-range".

Srujan Meesala: What are the prospects and challenges to scale current trapping technology to larger molecules?

KANG-KUEN:

1. In the scheme where we assemble molecules from atoms, using an assembling technique that bypasses the use of a Feshbach resonance would be important to generalize the kind of (larger) molecules that can be assembled. In my lab, we have some preliminary success in developing an all-optical assembling scheme that does not require a Feshbach resonance.
2. Because optical forces are weak, trapping molecules by optical means requires the molecules to be cooled below the trap depth (micro-Kelvin to milli-Kelvin). Laser cooling and optoelectrical cooling are two techniques that have been used to bring certain molecules into this temperature regime. For example, laser cooling of molecules up to 6 atoms have been recently demonstrated in John Doyle's lab. Cooling of larger molecules is also possible. Their scheme takes advantage of a metal atom in a molecule that serves as a photon cycling center and a ligand that can be bonded to the metal atom. "How general such a scheme is" is an exciting future work. There are also other types of traps, e.g. a deep superconducting magnetic trap in Ed Narevicious' lab and ion traps for molecular ions. Perhaps in the future, optical trap depths can also be increased dramatically.

Dietrich Leibfried: It seems like your lifetime does not match the theory within mutual 3-sigma. How does one have to interpret these uncertainties then? How can you claim agreement?

KANG-KUEN: Yes, I should be much more careful of claiming agreement. To me, a factor of 2 agreement was very good because previous calculations are different by an order of magnitude. However, for the factor of 2 "disagreement", this may point to the underlying assumption of ergodicity of the complex (for the RRKM calculation) not being true.

Stefan Spence: Thank you for your talk. Do you expect the isolation of single molecules, for example in optical tweezers, to provide further insights into these chemical interactions? What might be the requirements on the trapping potentials if you were to merge two molecules into the same optical tweezer?

KANG-KUEN: Yes and No. A cleaner "initial condition," such as having exactly two molecules for reaction/collision study, can help eliminate possible outcomes. But if there are multiple outcomes (including ones that we haven't thought about), then a direct probe is the best way to tease out the details. For an example of merging two molecules in the same optical tweezer for collision study, see the recent work by Cheuk, Anderegg et. al, arXiv:2002.00048 (2020)

(https://arxiv.org/abs/2002.00048).

The level of control you have over these molecules is very impressive. Could you say some more about the connections to chemistry (beyond synthesising new molecules), and what we can learn from these systems that is transferable (especially given that many experiments up to now were with Alkali atoms).

KANG-KUEN: A detailed understanding of this reaction (such as state-to-state reaction dynamics) requires comparison with theoretical calculations, which are not so easy for the level of accuracy we need and for such a reaction containing 4 heavy atoms. In fact, only calculations based on certain statistical assumptions can be made so far. Through this understanding, the refined theory can be used to understand other reactions. Other connections include detailed understanding of reaction intermediates which are central to all reactions without a reaction barrier and conservation of nuclear spins that we see in the bimolecular reaction of KRb.

What are the future prospects for impact on unsolved problems in Chemistry (or maybe one day even Organic chemistry?)

KANG-KUEN: There are many interesting unsolved problems in chemistry and for many of them, quantum mechanics does not play an important role. Our dream is to gain microscopic understanding (based on quantum mechanics) of chemical reaction. This will impact understanding of other reactions where quantum mechanics play an important role and serves as a foundation of understanding of reactions.

Based on your results and the results of your colleagues, do you think that there is any hope to find a simple polar molecule that is stable against ultracold chemistry, or is the decay you described universal?

KANG-KUEN: Yes, it is possible for molecules that consist of light atoms where the density of states of the reaction complex is expected to be much lower. But one would like to have many other desired properties such as a large dipole moment or large spaced internal levels of a chosen molecule beyond their collision properties. A more universal way of getting past two-body loss is to isolate individual molecules to prevent collisions using confining potentials or to modify their short-range interaction to provide repulsive forces such as microwave shielding. There are a number of theoretical proposals on microwave shielding and we await for experimental demonstration.

Is it possible to use the control techniques you have to protect polar molecules such as KRb from reaction losses in experiments?

KANG-KUEN: Yes, the loss I described in this talk came from collisions of pairs of molecules as the first step. Therefore, if the individual molecules are isolated, collisional loss is eliminated. This has been achieved by isolating molecules in optical lattices (in the case of KRb, this work was done in JILA).