

StereoAttoChemistry

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Steven Stolte studies the steric requirements of chemical processes. A reaction requires reorganization of atoms in the molecule(s) and Steven sought to understand this rearrangement in both space and time. We ask what happens when the atoms are not moving. This requires that we view the system with a very fine time resolution. Can such a fast time scale still be pertinent for chemistry? We discuss and demonstrate by computer simulations that it should be possible to induce interesting dynamics and that it is feasible to pump in a stereoselective fashion. We further show the photochemical implications of such novel processes.

Probing Translational Dynamics in Superfluid Helium Nanodroplets

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The photo-induced translational dynamics of species solvated in helium nanodroplets has been investigated with a variety of spectroscopic techniques. It has been found that for some solutes the interaction between with the helium environment changes upon electronic excitations from attractive to repulsive. As a result, the excited species are ejected from the droplets. Using ion imaging techniques, the speed distributions of the ejected atoms or molecules have been determined. The relation of these speed distributions to the critical Landau velocity, the velocity below which no energy and momentum can be transferred from a moving object to the superfluid helium environment, will be discussed. In order to address the role of the surface region, similar experiments have been performed involving species located on the surface of the droplets.

Quantum beat studies of angular momentum polarization in chemical processes.

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Chemical processes usually involve reactants and products that possess angular momentum, associated either with the spin and orbital motion of the electrons, or with the rotation of the nuclear framework of the molecule itself. Furthermore, the angular momentum of the products is often polarized during molecular photodissociation or chemical reaction. We are developing quantum beat spectroscopy as a method for probing angular momentum polarization based on laser induced fluorescence detection [1].

Applications of the method will be illustrated by reference to recent measurements of collisional depolarization cross-sections of OH(A) and NO(A) by a variety atomic and molecular species. These two systems provide an interesting comparison, and help elucidate the competing roles of kinematics and potential energy surface on the depolarization process. The results for collisions of the radicals with the rare gases are supported by detailed quantum mechanical and quasi-classical calculations on newly developed potential energy surfaces [2-4]. Applications of quantum beat spectroscopy to the study of angular momentum polarization effects in molecular photodissociation will also be discussed.

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Non-threshold, threshold and non-adiabatic behaviour of the key interstellar C + C₂H₂ reaction

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The C + C₂H₂ reaction is a key process in interstellar cloud chemistry. In a crossed-beam scattering experiment performed at eight collision energies between 0.44 and 4.5 kJ mol⁻¹ approaching those which characterize these low temperature environments, we determined differential cross-sections by detecting the H-atom product. The two channels leading to

cyclic and *linear* C₃H are clearly distinguished; the integral cross-section of the *c*-C₃H + H channel monotonically decreases with increasing relative translational energy whilst the *l*-C₃H + H channel exhibits a translational energy threshold. Moreover, comparison of the H-atom yields from the C + C₂H₂ and C₂H₄ reactions show that the C₃ + H₂ non-adiabatic channel dominates.

Novel approaches towards studying time-resolved molecular dynamics

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In the last few years two novel XUV/x-ray sources have emerged that allow to investigate time-resolved atomic and molecular dynamics in a very new way. On the one hand, attosecond laser sources that are based on the process of high-harmonic generation, provide a means to perform time-resolved measurements on electronic timescales. In my talk I will present a first example of the application of attosecond light sources towards a study of time-resolved molecular electron dynamics. On the other hand, emerging XUV/x-ray Free Electron lasers, such as the FLASH laser in Hamburg and the LCLS in Stanford, allow the development of novel strategies for the elucidation of time-resolved molecular dynamics that are based on diffraction. I will present results from recent experiments at FLASH that are geared towards this goal.

Velocity map imaging studies of inelastic scattering of polyatomic molecules

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Over the past decade, gas-phase inelastic scattering experiments using velocity map imaging have reached a high level of sophistication. Investigations of the scattering of diatomic molecules with rare gas atoms provide state-to-state collision cross sections from which information about the potential energy surface and the dynamics of the intermolecular interactions can be extracted. In this talk imaging studies of the scattering of polyatomic molecule with diatomic molecular partners will be described. An important example which is relevant in astrophysics is the inelastic collision of NH_3 and H_2O with H_2 . These collisions result in the anomalous non-thermal emission of NH_3 microwave radiation which has been observed in interstellar clouds¹, *i.e.*, the emitting molecules are excited by collisions with very abundant surrounding interstellar molecules such as H_2 or He, followed by spontaneous or stimulated emission. Previous work on the water system includes differential cross sections measurements by for the $\text{H}_2\text{O} + \text{He}$ scattering system by Brudermann *et al*² and by Cappelletti *et al*³ and state-to-state integral cross sections for $\text{H}_2\text{O} + \text{Ar}$ by Chapman *et al*⁴.

In this talk state-to-state inelastic scattering experiments of ND_3 and H_2O with Ar, He, or H_2 using a crossed-beam velocity map imaging apparatus will be described. From the

experimental images, differential state-to-state collision cross sections (DCS) are acquired and compared to theoretical calculations. Our DCS results show very anisotropic product angular distributions after inelastic collisions, which had not been considered in previous experiments. DCS provide detailed information about the anisotropies of potential energy surfaces of intermolecular interactions. In addition to DCS, relative integral state-to-state collision cross sections can be obtained from our experimental images. The integral cross sections are used in databases for astrophysical models. Propensity rules of rotational transitions for H₂O and ND₃ collisions are also obtained.

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³ D. Cappelletti, V. Aquilanti, E. Cornicchi, M. M. Teixidor, and F. Pirani, *The Journal of Chemical Physics* **123**, 024302 (2005).

⁴ W. B. Chapman, A. Kulcke, B. W. Blackmon, and D. J. Nesbitt, *The Journal of Chemical Physics* **110**, 8543 (1999).

UV spectroscopy of gas phase proteins and metal cluster-peptide hybrids

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We perform gas phase experiments on biomolecules with the objective of providing the bases to construct atomic models of functional biomolecule in actions. The experimental set up integrates an electrospray ion source, an ion trap mass spectrometer and one or two tunable UV-Vis lasers. A first series of results was obtained on multiply negatively charged peptides and proteins. For polyanions, electron emission is observed after irradiation. Electron detachment yield as a function of laser wavelength and optical fingerprints of proton and radical transfers will be presented. Metal nanoparticles are currently used as labels for optical detection and imaging of biomolecules. We will show that gas phase experiments can be used to determine the exact nature of the binding between a metal particle and a peptide, and the influence of the metal part on the conformation of the biomolecule. The coupling between the surface plasmon resonance of the metal moiety and the excited states of the peptide will also be discussed.