CFEL SCIENCE

SEMINAR

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CFEL – Building 99, seminar room III (ground floor)

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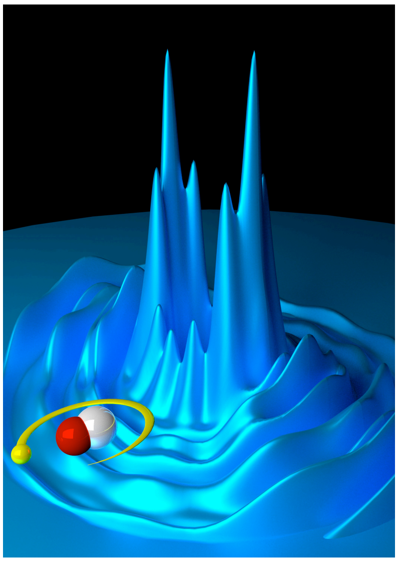
Unraveling Molecular Collisions

Molecular scattering processes play an important role in the interstellar medium, atmospheres and combustion. To fully understand these processes, accurate theoretical models are required, which have to be tested extensively. In our joint experimental and theoretical project, high-resolution scattering experiments are used to test the quality of state-of-the-art theory.

The combination of a Stark decelerator and Velocity Map Imaging is a powerful tool to study molecular collisions. It allows us to perform scattering experiments with unprecedented resolution, revealing details of molecular collisions that are washed out otherwise. Using these techniques, we were able to resolve quantum diffraction oscillations in differential cross sections for inelastic collisions between NO radicals and rare gas atoms [1]. The cross sections were in excellent agreement with the results from quantum close-coupling scattering calculations based on intermolecular potential energy surfaces. The observation of the diffraction oscillations provides a sensitive test for the accuracy of the potentials used [2,3].

Especially at low temperatures, scattering resonances occur at specific energies at which the colliding particles temporarily form quasi-bound complexes, resulting in peaks in integral collision cross sections. Moreover, dramatic changes are predicted in the angular distribution of the collision products as function of energy around these resonances. It has proven extremely challenging to measure these resonances and angular distributions. Our high-resolution experiment has facilitated the observation of resonance fingerprints in the state-to-state differential cross sections for inelastic collisions between NO molecules and He atoms [4]. The measurements were in excellent agreement with scattering calculations, with which we could fully characterize the resonances. This combination of experiments and theory allowed us to study how resonances affect the angular distribution of the scattered molecules. This provides new information on the quantum character of molecular collisions. Moreover, resonances can be an excellent test for the quality of the potential energy surfaces used in the scattering calculations.



"Illustration of the scattering wavefunction for collisions between nitric oxide (NO) molecules and helium (He) atoms at a resonant collision energy. The collision partners form a quasi-bound complex and stick together longer than the normal fly-by time."

[1] A. von Zastrow, J. Onvlee, S. N. Vogels, G.C. Groenenboom, A. van der Avoird, and S.Y.T. van de Meerakker, *Nature Chemistry* **6**, 216 (2014) [2] S.N. Vogels, J. Onvlee, A. von Zastrow, G.C. Groenenboom, A. van der Avoird, and S.Y.T. van de Meerakker, *Phys. Rev. Lett.* **113**, 263202 (2014) [3] J. Onvlee, S.N. Vogels, A. van der Avoird, G.C. Groenenboom, and S.Y.T. van de Meerakker, *New J. Phys.* **17**, 055019 (2015) [4] S. N. Vogels, J. Onvlee, S. Chefdeville, A. van der Avoird, G.C. Groenenboom, and S.Y.T. van de Meerakker, *Science* **350**, 787 (2015).

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