Molecular Systems group

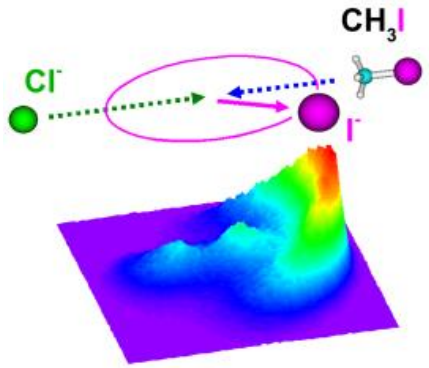
Our research focus:
Quantum effects in the structure and interaction of molecules and ions

universität innsbruck

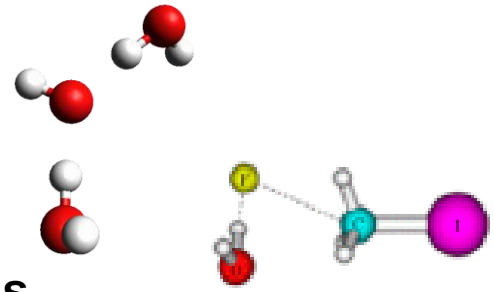
Molecular Systems

Dynamics and Spectroscopy of Charged Molecular Systems

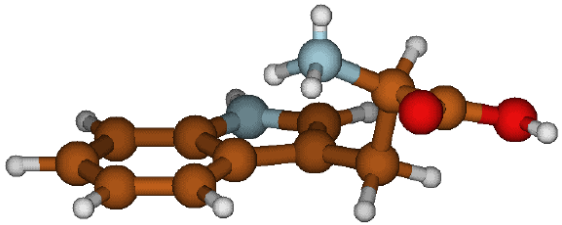
Ion-molecule reaction dynamics



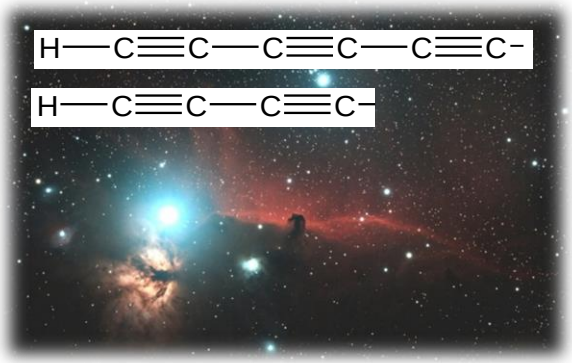
Micro-hydration effects



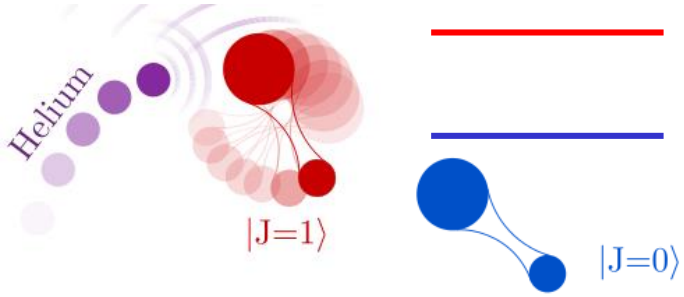
Biomolecular ions



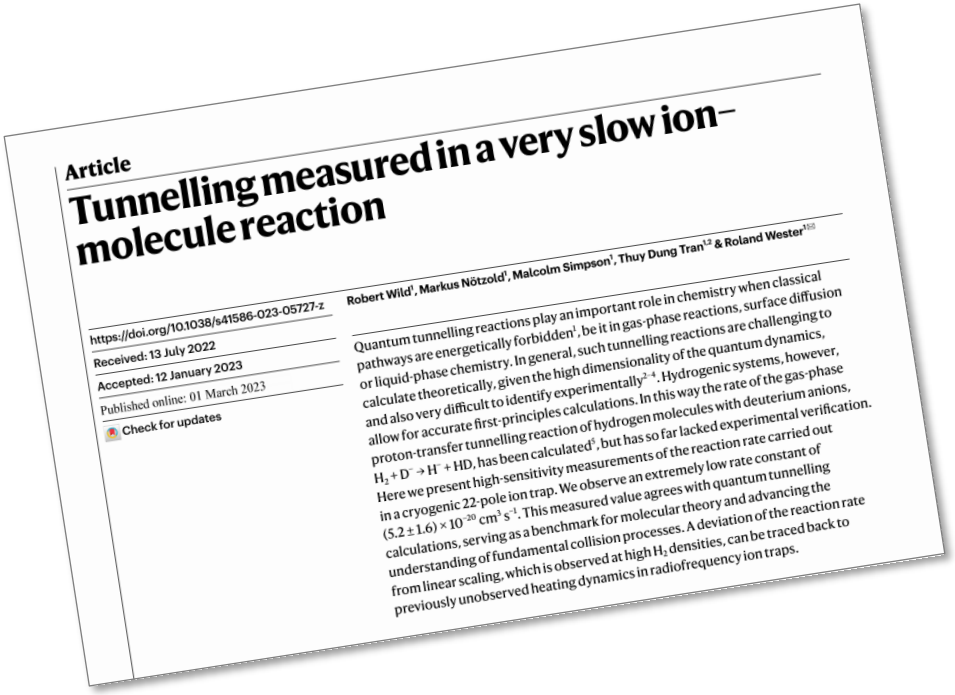
Interstellar ion formation



Cold and state-controlled ions



Recent Breakthrough: Quantum tunneling in the $D^- + H_2$ reaction



Article

Tunnelling measured in a very slow ion–molecule reaction

Robert Wild[1], Markus Nötzold[1], Malcolm Simpson[1], Thuy Dung Tran[1,2] & Roland Wester[1]✉

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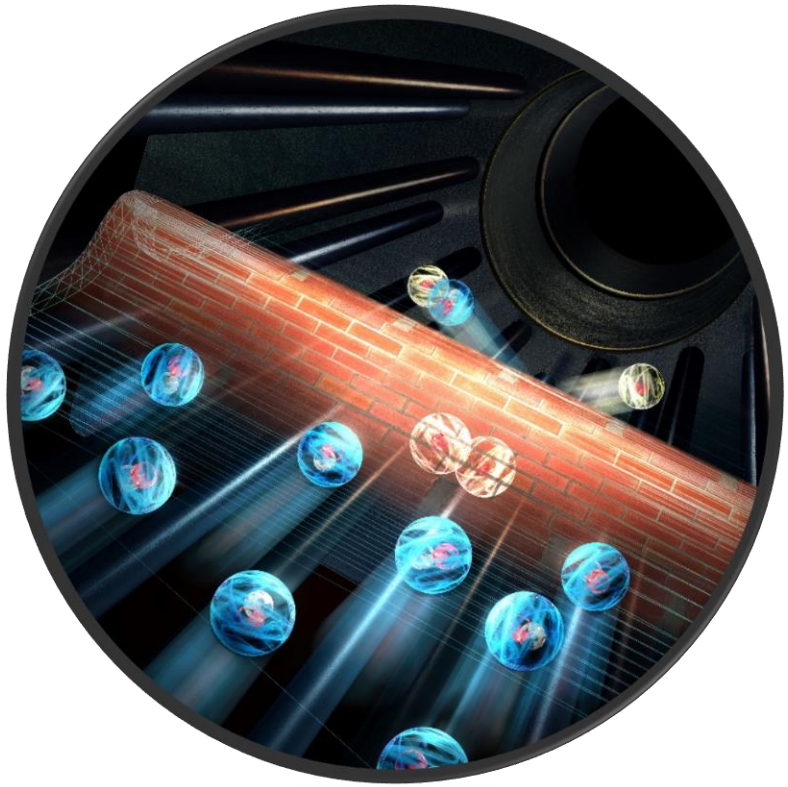
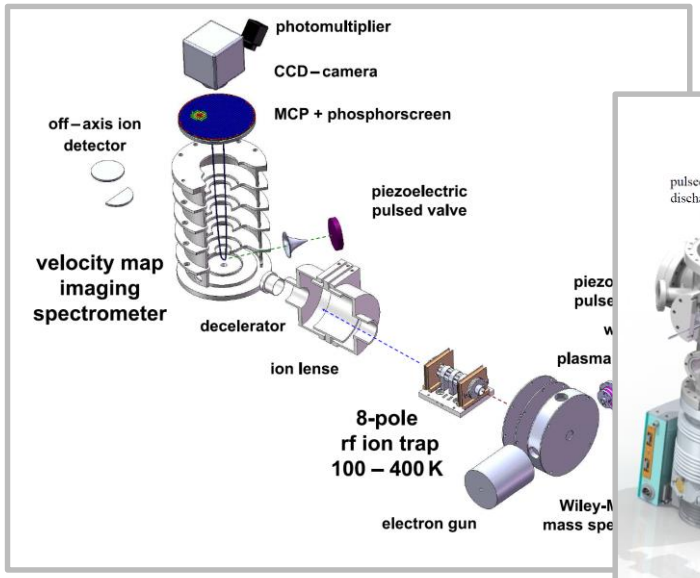
Quantum tunnelling reactions play an important role in chemistry when classical pathways are energetically forbidden[1], be it in gas-phase reactions, surface diffusion or liquid-phase chemistry. In general, such tunnelling reactions are challenging to calculate theoretically, given the high dimensionality of the quantum dynamics, and also very difficult to identify experimentally[2–4]. Hydrogenic systems, however, allow for accurate first-principles calculations. In this way the rate of the gas-phase proton-transfer tunnelling reaction of hydrogen molecules with deuterium anions, $H_2 + D^- \rightarrow H^- + HD$, has been calculated[5], but has so far lacked experimental verification. Here we present high-sensitivity measurements of the reaction rate carried out in a cryogenic 22-pole ion trap. We observe an extremely low rate constant of $(5.2 \pm 1.6) \times 10^{-20}$ cm^3 s^{-1}. This measured value agrees with quantum tunnelling calculations, serving as a benchmark for molecular theory and advancing the understanding of fundamental collision processes. A deviation of the reaction rate from linear scaling, which is observed at high H_2 densities, can be traced back to previously unobserved heating dynamics in radiofrequency ion traps.



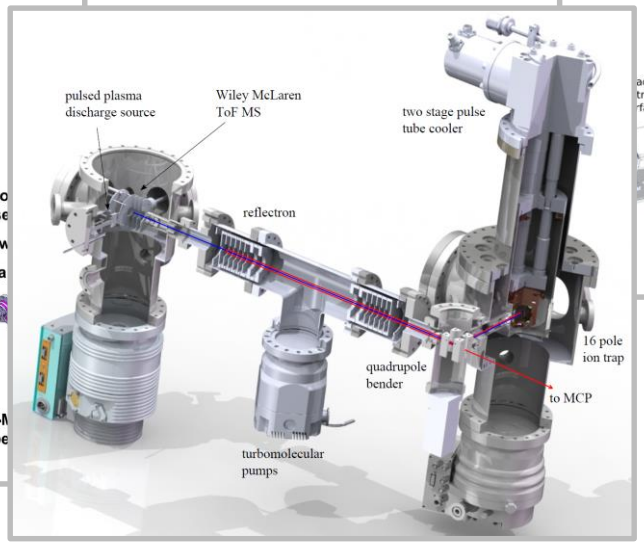
R. Wild *et al.*, Nature (2023)

Dynamics and Spectroscopy of Charged Molecular Systems

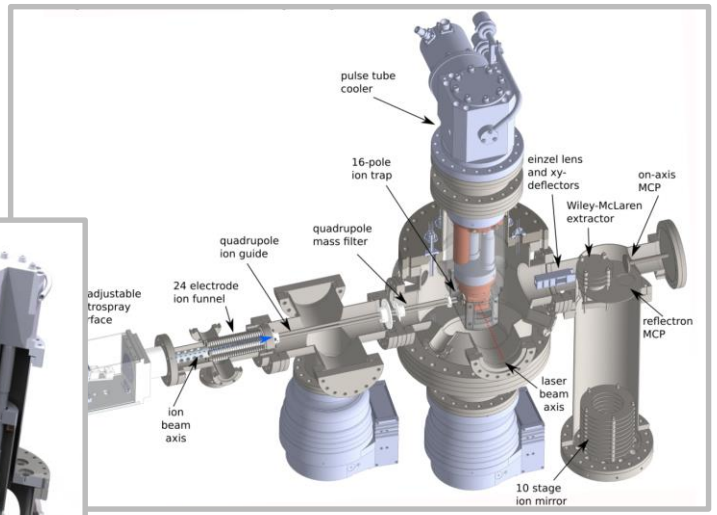
Experimentelle Aufbauten



Kreuzstrahlspektrometer für Ionen-Molekül-Reaktionsdynamik



6 Kelvin Ionenfalle für Laborastrophysik an interstellarer Ionen

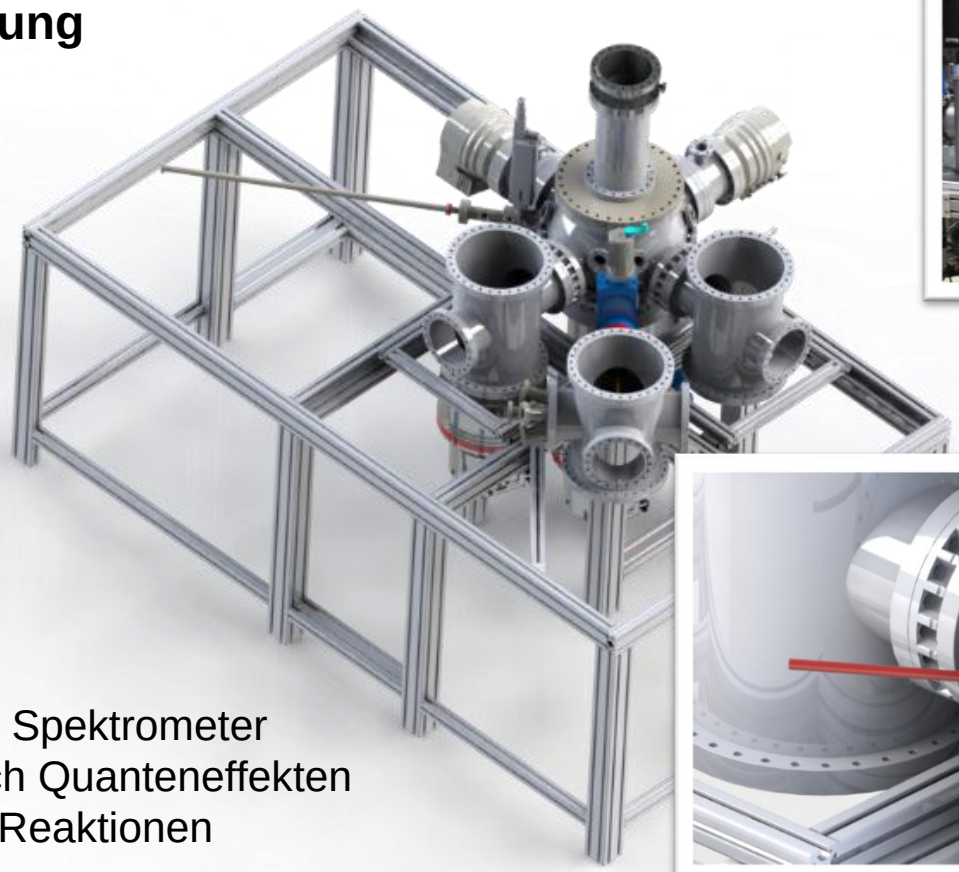


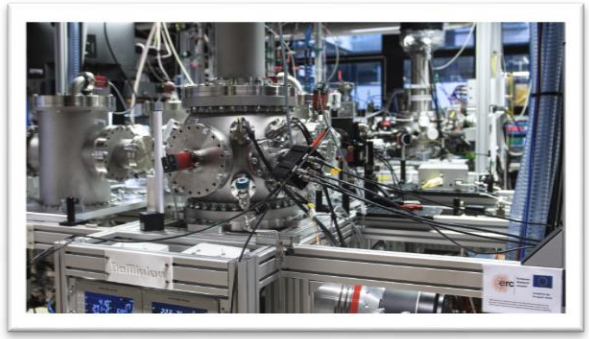
3 Kelvin Elektrospray-Ionenfalle für Spektroskopie an Biomolekülen und Clustern

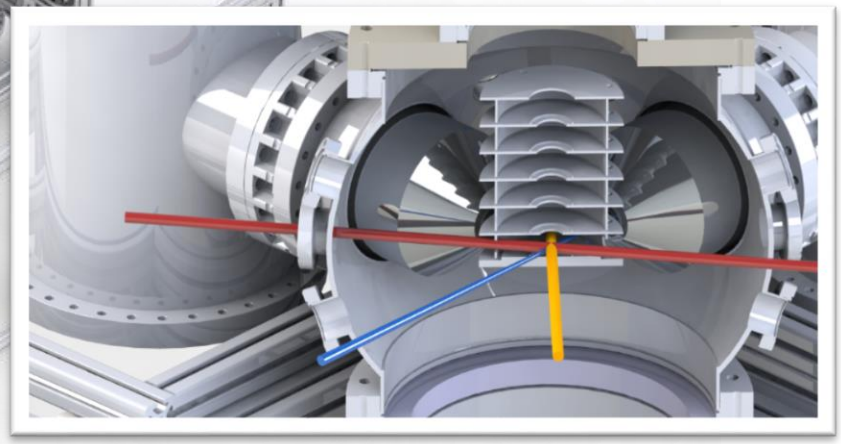
Dynamics and Spectroscopy of Charged Molecular Systems

Neue Entwicklung

DoMInIon





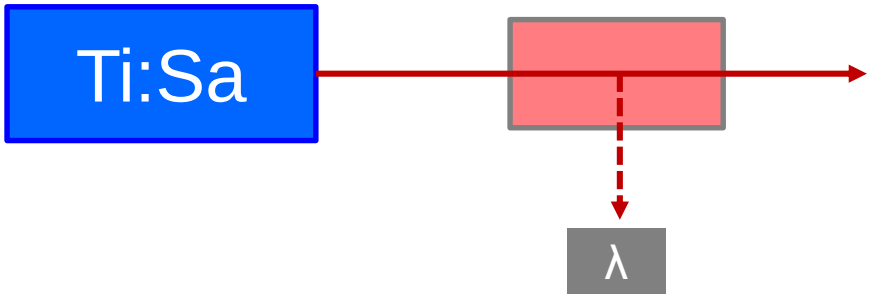


Hochauflösendes Spektrometer
für die Suche nach Quanteneffekten
in Ionen-Molekül-Reaktionen

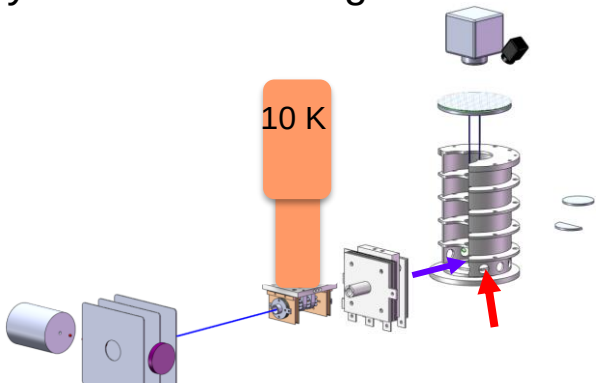
Dynamics and Spectroscopy of Charged Molecular Systems

Mögliche Themen für Bachelorarbeiten 2025

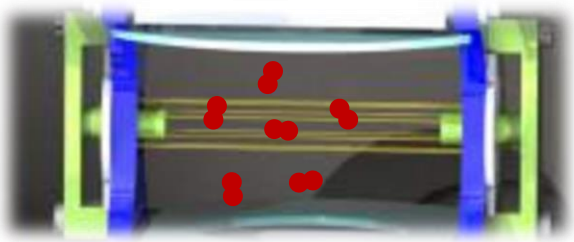
Aufbau einer Raman-Spektroskopie für p-H_2



Ein Kryostat für Streuung von kalten Ionen



Ionen-Molekül-Reaktionen mit p-H_2



Charakterisierung einer hoch-sensitiven EMCCD-Kamera

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Dynamics and Spectroscopy of Charged Molecular Systems

Bei Interesse, einfach melden:

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Vielen Dank für die Aufmerksamkeit!

Atoms, Light, and Molecules
Innsbruck Physics Research Center

FWF

erc

Collaborations

Szeged
Heidelberg
Prag
Stockholm
Bordeaux
Orlando
Albuquerque