Colloquium

SFB 956

Conditions and Impact of Star Formation

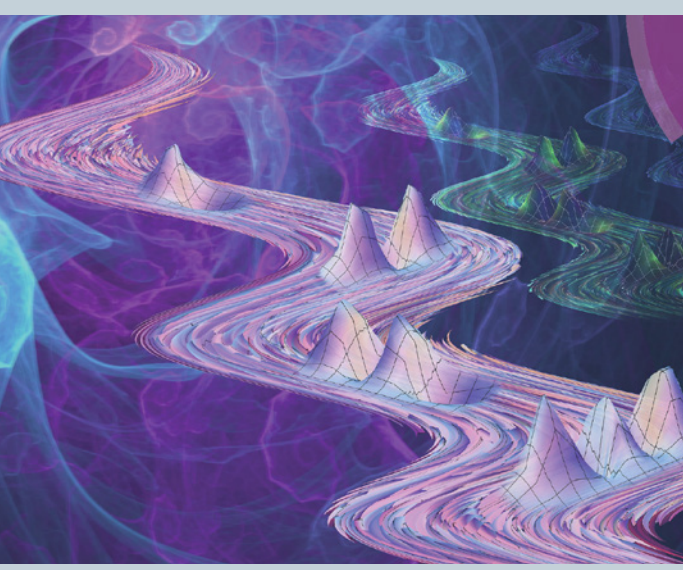
16.10.2017

Monday 3:00 pm

Physikalische Institute Köln

Lecture Hall III

Zülpicher Straße 77 | 50937 Köln



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Cations in Motion

The notion of molecules and structures is central to our chemical understanding of the nature surrounding us. One useful definition of neutral as well as charged molecules is that they correspond to minima on potential energy surfaces (PES) and the local PES must support at least one bound rovibrational state. The structure of a molecule is usually considered to be the geometry corresponding to the minimum. If a molecule exists and has a structure, it is also commonly accepted that its internal motions can be separated into vibrations and rotations, motions which usually have very different time and energy scales.

Nevertheless, there are chemical systems where both the notion of a molecule, that of a structure, as well as the separation of rotational and vibrational motion can be questioned. One part of the present lecture is centered around cations where the concept of a structure and the separation of vibrations and rotations seems to break down. Notably, cations characterized by bonds whereby the covalent bonding picture is challenged are prone to exhibit unusual structures and unusual quantum dynamical behavior. Highly excited states of "simple" molecules also exhibit unusual rotational-vibrational characteristics but in the cases of quasistructural cations it is not sufficient to keep the concept of a well-defined structure to explain the high-resolution spectrum of the molecule.

The lecture focuses on the following cations and their deuterated analogues: H_3^+, HeH_2^+, $ArNO^+$, H_5^+, and CH_5^+. Not only bound but also rovibrational resonances are investigated for some of these cations. Fourth-age quantum chemical tools developed to understand the complex quantum dynamics of these cationic systems are presented and discussed briefly.