Julius-Maximilians-
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Kolloquium der Physikalischen und Theoretischen Chemie

Dienstag, 26.06.2018 **Hörsaal D, Chemiezentralgebäude, 17:15 Uhr**

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Titel: Big quantum effects in small molecules

Abstract:

We discover surprising consequences of the well-known quantum effects such as zero-point energies, superposition and interferences of quantum states, tunneling, and constraints imposed by nuclear spins. The examples include a new type of chemical bonding: "vibrational bonding" stabilizes BrMuBr at its low, broad transition state due to the reduction of vibrational zero point energies (Muonium Mu is the light isotope of hydrogen, $m_{Mu} = m_H/9$).[1] The large mass ratio enables another effect in molecules such as FHF^-, CdH_2 or OsH_4: well designed circularly polarized laser pulses excite superpositions of degenerate bending or stretching states with strong ring currents of the highly charged nuclei that induce very strong intra-molecular magnetic fields (> 600 T).[2] By analogy, one can prepare molecules such as Mg-porphyrine in interfering ground and degenerate excited electronic states with strong electronic fluxes (about 1 e/fs, 1 fs = 1 femtosecond = 10^{-15} s).[3] Analogous preparation of interfering electronic states in molecular ions such as H_2^+ or $HCCI^+$ yield electronic fluxes that support periodic charge migration from one molecular end to the other, on time scale of few hundred as (1 as = 1 attosecond = 10^{-18} s).[4,5] Laser control of multidirectional charge migration is simulated for C_6H_6.[6] The laser pulse breaks electronic structure symmetry. Symmetry can be restored by a second pulse (= (time-reversed) copy of the first pulse), with few attosecond precision of the time delay, also confirmed experimentally for the Rb atom.[7] - Likewise, interfering nuclear ground and excited states yield circular and linear tunneling, e.g. in the model $B_2Cl_2F_2$ and NH_3 molecules; here, analogous time evolutions of the nuclear densities correlate with entirely different tunneling fluxes.[8] Electrons may flow with the nuclei, or in oblique directions (example: rhomb-to-rhomb isomerization of B_4);[9] transient antagonistic electronic fluxes cause electronic restructuring at transition states (example: Na_2 in excited state with double well potential).[10] Antagonistic nuclear fluxes in vibrating Na_2 give rise to the "quantum accordion effect".[11] Finally, the nuclear spin statistics theorem implies surprising quantum effects in systems such as the planar boron rotors $^{11}B_{11}^-$, $^{11}B_{13}^+$ etc.[12] For example, one may of course calculate their global minimum structures (GM), but it is impossible to prepare them in GM.[13]

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