Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

Kolloquium der Physikalischen und Theoretischen Chemie

Dienstag, 25.10.2016 **Hörsaal D, Chemiezentralgebäude, 17:15 Uhr**

Sprecher: Uwe Manthe

(Universität Bielefeld)

Titel: High-dimensional quantum dynamics of reactive processes

Abstract:

The accurate description of the quantum dynamics of polyatomic systems is a challenging subject. The present talk focuses on theoretical concepts for the simulation and analysis of polyatomic reaction processes and presents prototypical applications.

The scaling of the numerical effort with dimensionality is a key problem of quantum dynamics calculations studying polyatomic systems. The multiconfigurational time-dependent Hartree (MCTDH) approach and it multi-layer extension have been established as efficient schemes for the accurate treatment of high-dimensional systems. In the present talk, the fundamental ideas of the approach are introduced and discussed.

The quantum transition state approach provides an intuitive framework for the accurate description of reactions proceeding via a potential barrier. It is typically used to study reaction rates. In recent work, the theory has extended to the calculation of fully state-resolved reaction probabilities and cross-sections. The reactive scattering is separated into two half-collisions starting from the transition state region and generalized flux correlation functions are used to rigorously compute fully state-resolved scattering matrix elements from the simulation data. In this talk, the theoretical concept is introduced and accurate results obtained for the
$H+CH_4 \rightarrow H_2+CH_3$ reaction are presented. The ro-vibrational control of the chemical reactivity is discussed in the context of the Polanyi rules and the correlation between the quantum states of the reactants and products is analyzed.

Ultrafast intermolecular rearrangements in fluxional molecules and clusters results in specific effects not seen in rigid or semi-rigid molecules. Here it will be shown that fundamental symmetry arguments require the complete breakdown of the separability of rotational and internal motion in fluxional system of the type AB_n or B_n with $n > 4$. Rotational and internal motion must always be entangled. Numerical results for a prototypical example, the CH_5^+ molecular cation, will be shown.

Organisation: V. Engel

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Weitere Informationen unter:
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