Julius-Maximilians-
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Kolloquium der Physikalischen und Theoretischen Chemie

Dienstag, 31.05.2011 **Hörsaal D, Chemie Zentralbau, 17:15 Uhr**

Sprecher:

Peter Vöhringer

Universität Bonn

Thema:

Multidimensional vibrational resonance: An infrared window to hydrogen bond dynamics.

Abstract:

In general, the high-frequency intramolecular D−H stretching vibration of a hydrogen-bonded donor(D)-acceptor(A) pair, D−H···A, couples to the intermolecular D···A restricted translations and hence, to the hydrogen-bond bending and stretching modes of the pair. We exploit this correlation using two-dimensional infrared (2DIR) spectroscopy to study the dynamics of vibrational energy flow and equilibrium structural relaxations in polyatomic systems exhibiting hydrogen-bond networks with various degrees of complexity. (i) We use diastereomeric poly-alcohols as low-dimensional model systems for the vibrational dynamics and spectroscopy of random hydrogen-bonded networks of associated liquids and fluids such as bulk water and ammonia. Such systems provide unequivocal evidence of the excitonic couplings between neighboring OH's contributing to the H-bond wire or H-bond network, respectively. (ii) Supramolecular host-guest complexes like crown ether hydrates feature a small H-bond network that is spatially confined to the concave cavity of the receptor. Conformational transitions within the receptor perturb this network and can therefore be probed through 2DIR spectroscopy on the intramolecular stretching modes of the substrate.

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Weitere Informationen unter
http://www.phys-chemie.uni-wuerzburg.de