

AGGREGATION OF SMALL MOLECULES – FOR618 SYMPOSIUM – MAY 29 – 31 – PROGRAM

Day	Time	Speaker	Topic
29.05.	18:00 - 19:30	Welcome Reception	
	19:30 - 20:15	Stefan Grimme	"Dispersion Corrected Density Functional Theory"
	20:15 - 21:00	Friedrich Temps	"Noncovalent Interactions in the Ultrafast Dynamics of Electronic Excited DNA Building Blocks"
30.05.	09:00 - 09:45	Wolfgang Domcke	"Ultrafast Nonadiabatic Photochemistry of Hydrogen Bonds in Organic and Biological Chromophors"
	09:45 - 10:30	Manfred Kappes	The periodic table at 55 (and some structures of other atomic cluster sizes)
	10:30 - 11:00	Coffee break	
	11:00 - 11:30	Martina Havenith-Newen	Rock and Roll at 0.37 K
	11:30 - 12:00	Dominik Marx	"Aggregation-Induced Chemical Reaction: HCl-Water Aggregates in the Gas Phase and in Superfluid Helium"
	12:00 - 13:00	Lunch	
	13:00 - 13:45	Mark Johnson	"Capturing Reaction Intermediates with Cryogenic Ion Spectroscopy"
	13:45 - 14:15	Georg Jansen	"Properties of Small Molecular Aggregates from Analytical Model Potentials obtained through Quantum Chemistry"
	14:15 - 14:45	Coffee break	
	14:45 - 15:30	Pavel Hobza	"Noncovalent Interactions: QM and MM approaches"
	15:30 - 16:00	Nikos Doltsinis	Simulating aggregation from first principles
	16:00 - 16:30	Coffee break	
	16:30 - 17:15	Gautam Desiraju	The Structural Landscape in Crystal Engineering
	17:15 - 17:45	Klaus Merz	"The Importance of Deuterium and Fluorine-Substituents on Molecular Aggregation Processes"
	17:45-18:15	Roland Boese	Crystalline Organic Hydrates - Frozen Stages of the Dissolution Process?
31.05.	09:00 - 09:45	Christopher Hunter	"The Anatomy of Complex Recognition Interfaces"
	09:45 - 10:30	Gary E. Douberly	"Radical Containing Clusters in Helium Nanodroplets"
	10:30 - 10:45	Coffee break	
	10:45 - 11:15	Karl Kleinermanns	"Isomer Selective Vibronic Spectroscopy of Benzene-Acetylene Clusters – Towards a Better Understanding of Seed Crystal Formation"
	11:15 - 11:45	Karina Morgenstern	Aggregation of molecules on surface: From coverage to chirality dependence
	11:45 - 12:15	Wolfram Sander	Aggregation and Solvation of Radicals and other Reactive Intermediates