

## Schedule International Symposiums “Small Molecules in Interactions”

### March 26, 2012

From 8.00	Registration	
09.45-10.00	Opening of Symposium	
10.00-10.30	Gautam R. Desiraju	Halogen bonding in crystal engineering
10.30-11.00	Andrzej Katrusiak	Intermolecular interactions in compressed crystals
11.00-11.30	Oleg V. Shishkin	Supramolecular architecture of molecular crystals derived from topology of intermolecular interactions
11.30-12.00	Oral Poster Presentation	
12.00-13.00	Lunch	
13.00-13.30	Angshuman R.Choudhury	Study of weak interactions in halogen substituted diphenylmethanimine and diphenyldiazenes
13.30-14.00	T. N. Guru Row	Charge density analysis of intermolecular interactions from supramolecular synthons
14.00-14.30	Vera Vasylyeva	Influence of weak directing substituents on molecular aggregation
14.30-15.00	Dmitry Yufit	Low-melting molecular complexes of methyl halides – halogen bonding makes the difference
15.00-16.00	Coffee break & Poster Session	
16.00-16.30	Christof Hättig	Explicitly-correlated wavefunction methods: New perspectives for <i>ab initio</i> studies on intermolecular interactions
16.30-17.00	George Pitsevich	The argon matrix affects on internal rotation barriers and torsional states of CH <sub>3</sub> OH
17.00-17.30	Valeriy Pogorelov	H-bond clustering of small molecules isolated in low temperature argon matrix
17.30-18.30	Poster Session	
19:00 -	Conference Dinner	

### March 27, 2012

9.00-9.30	Roland Boese	Supramolecular synthesis – co-crystallization of small molecules
9.30-10.00	Christian Lehmann	Preparation and structure determination of diastereomeric co-crystals
10.00-10.30	V. R. Pedireddi	Molecular recognition studies of cyanuric and trithiocyanuric acids
10.30-11.00	Coffee break	
11.00-11.30	Agata Bialonska	Solid solutions of brucinium diastereomeric salts with <i>N</i> -(3-nitrobenzoyl)-amino acid
11.30-12.00	Michael Mastalerz	Defined organic molecules for permanent porous crystals
12.00-12.30	Andrew D. Bond	Rediscovering polytypism in molecular crystals
12.30-13.30	Lunch	
13.30-16.00	Exhibitions	
16.00-16.30	Rochus Schmid	Towards first principles derived force fields for host-guest interactions in porous hybrid materials
16.30-17.00	Detlef W. M. Hofmann	Fast estimation of the free energy of synthons by data mining
17.00-17.30	Tatiana E. Gorelik	Electron diffraction on molecular crystals
17.30-17.45	Closing of Symposium	

Location: Ruhr-University Bochum, Veranstaltungszentrum (VZ), Level 04, Hall 3

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