

Interdisciplinary Symposium: Chemical concepts and Quantum Chemistry

Nov 18 – 20, 2019
Mathematikon, Heidelberg, Germany
Im Neuenheimer Feld 205
69120 Heidelberg

Overview I			
	Monday, Nov 18	Tuesday, Nov 19	Wednesday, Nov 20
9:00		Chemical Bonding III	Chemical Concepts I
9:50			
10:40		Break	Break
11:10	Introduction	Molecular Structure	Chemical Concepts II
12:00			Discussion
12:50	Welcome reception	Lunch	End of symposium
14:00	Chemical Bonding I	Orbitals	
14:50			
15:40	Break	Break	
16:10	Chemical Bonding II	Models and Photons	
17:00			
17:50	Dinner	Dinner	



UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386



Overview II			
	Monday, Nov 18	Tuesday, Nov 19	Wednesday, Nov 20
9:00		Georg Jansen	Frank De Proft
9:50		Arne Lüchow	Clémence Corminboeuf
10:40		Break	Break
11:10	Marcus Elstner	Markus Reiher	Andreas Dreuw
12:00	Sebastian Höfener	Robin Hendry	Discussion
12:50	Welcome reception	Lunch	End of symposium
14:00	Paul Needham	W. H. Eugen Schwarz	
14:50	Gernot Frenking	Jochen Autschbach	
15:40	Break	Break	
16:10	Ángel Martín Pendás	Rafaela Hillerbrand	
17:00	Célia Fonseca Guerra	Jan-Peter Meyn	
17:50	Dinner	Dinner	

Each speaker has a time frame of 50 minutes, of which 10 minutes should be reserved for discussion.

Monday, Nov 18		
Introduction		
11:10	Marcus Elstner	Quantum Chemical Concepts
12:00	Sebastian Höfener	Chemical Bonding
12:50	Welcome reception	
Chemical Bonding I		
14:00	Paul Needham	Some Topics in the Philosophy of Chemistry
14:50	Gernot Frenking	The Chemical Bond and the Atomic Valence Space
15:40	Break	
Chemical Bonding II		
16:10	Ángel Martín Pendás	Counting Electrons in Atoms (within Molecules): new Models, new Insights?
17:00	Célia Fonseca Guerra	Hydrogen Bonding explained: the Synergistic Power of Energy Decomposition Analysis and Molecular Orbital Theory
17:50	Dinner	

Tuesday, Nov 19		
Chemical Bonding III		
9:00	Georg Jansen	The strength of Weak Interactions: Computing and Modeling Intermolecular Forces
9:50	Arne Lüchow	Insight into Chemical Bonding from Topological Analysis of the many-electron Probability Density
10:40	Break	
Molecular Structure		
11:10	Markus Reiher	Molecular Structure from an All-Particle Pre-Born-Oppenheimer Perspective
12:00	Robin F. Hendry	Molecular Structure as an Emergent Phenomenon
12:50	Lunch	
Orbitals		
14:00	W. H. Eugen Schwarz	What is real in Reality and in Observations of Molecules?
14:50	Jochen Autschbach presented by W. H. Eugen Schwarz	Orbitals and Chemical Bonding - some Fiction and some Facts
15:40	Break	



UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386



Models and Photons		
16:10	Rafaela Hillerbrand	The Role of Scientific Models as Mediators between Theory and Experiment
17:00	Jan-Peter Meyn	What are Photons, and why do we need them?
17:50	Dinner	

Wednesday, Nov 20		
Chemical Concepts I		
9:00	Frank De Proft	Density Functional Theory based Chemical Concepts: Prospects, Issues and recent Developments
9:50	Clémence Corminboeuf	Quantification of Fuzzy Chemical Concepts
10:40	Break	
Chemical Concepts II		
11:10	Andreas Dreuw	Quasi-Particles in Chemistry
Discussion		
12:00	N.N.	
12:50	End of symposium	