

## Contacts to and within molecules

### Program

**Wednesday, September 19**

9:00 – 9:10 Welcome remarks

#### *Coupling within molecules A*

9:10 – 9:50 Felix Tuczek Christian-Albrechts-Universität zu Kiel  
Spin-State Switching of Iron and Nickel Complexes in Homogeneous Solution and on Surfaces

9:50 – 10:30 Guillem Aromí Universitat de Barcelona  
Molecular Prototypes for Spin-Based CNOT Quantum Gates

#### *Coupling within molecules B*

10:50 – 11:30 Christoph Jacob Karlsruher Institut für Technologie  
Subsystem quantum chemistry for describing contacts to and within molecules

11:30 – 11:50 Alejandra Escribano Universität Hamburg  
Photochromic Molecular Switches Connecting Paramagnetic Metallocenes

11:50 – 12:30 Johannes Neugebauer Technische Universität Braunschweig  
Calculation of excited states in extended systems from selective and subsystem time-dependent DFT

#### *Coupling within molecules C*

14:30 – 15:10 David Schultz North Carolina State University  
Evaluating bridge-dependent electronic coupling via exchange couplings and hyperfine coupling constants in metal complexes of donor-bridge-acceptor biradicals

15:10 – 15:30 Carmen Herrmann Universität Hamburg  
Electronic communication through molecular bridges in coupled spin systems and molecular electronics

15:30 – 16:10 Boris LeGuennic Université de Rennes 1  
Addressing magnetic and conduction properties through weak-bond networks: ab initio inspections

16:10 – 16:30 Bernhard Bugenhagen Universität Hamburg  
Synthesis of and magnetic coupling in covalently linked complex chains

***Molecules on surfaces A***

- 16:50 – 17:30 Marc Tornow Technische Universität Braunschweig  
Electronic properties of novel organophosphonate layer architectures on silicon substrates
- 17:30 – 17:50 Annik Abel Universität Hamburg  
Redox-active molecules as a functional surface on nanostructures
- 17:50 – 18:30 Andrea Cornia Università degli Studi di Modena e Reggio Emilia  
Chemical design, structure and magnetic response of gold-wired Single-Molecule Magnets

**Thursday, September 20**

***Molecules on surfaces B***

- 9:00 – 9:40 Hubertus Marbach Friedrich-Alexander-Universität Erlangen-Nürnberg  
Surface science with porphyrins: towards the rational design of functional molecular architectures
- 9:40 – 10:00 Jens Brede Universität Hamburg  
Spin resolved measurements of magnetic molecules on surfaces
- 10:00 – 10:20 Régis Decker Universität Hamburg  
Atomic-scale magnetism of cobalt-intercalated graphene

***Transport through molecules***

- 10:40 – 11:20 Herre S. J. van der Zant TU Delft  
Molecular signatures in transport: interference and charging effects
- 11:20 – 11:40 C. Klinke Universität Hamburg  
Supramolecular interaction of singlewall carbon nanotubes with a functional tetrathiafulvalene-based mediator for iodine sensitive field effect transistors
- 11:40 – 12:20 Mario Ruben Karlsruher Institut für Technologie  
Supramolecular Quantum Spintronics
- 12:20 – 12:40 Michael Karolak Universität Hamburg  
Geometry and Ligand controlled Kondo Effect in Molecular Nanosystems