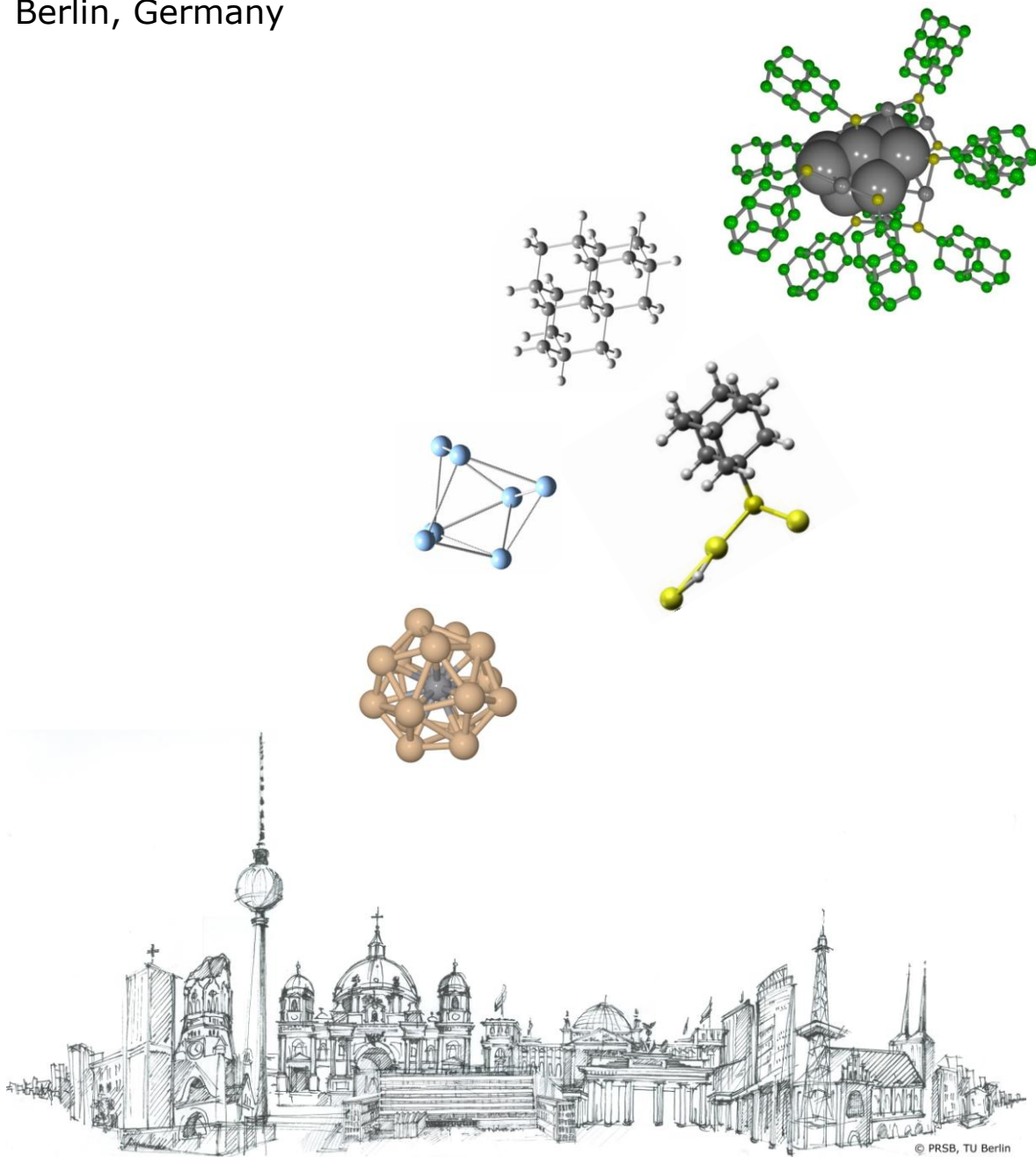


International Symposium Research Unit 1282 (FOR 1282)

## **Controlling the Electronic Structure of Semiconductor Nanoparticles by Doping and Hybrid Formation**

February 22-24, 2017

Berlin, Germany



Wednesday, February 22<sup>nd</sup>

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12:00	Registration, Catering
13:20-13:30	THOMAS MÖLLER (TU Berlin, Germany) Opening remarks
13:30-14:10	PETER LIEVENS (University of Leuven, Belgium) The challenge of knowing how a cluster looks like: elemental and doped germanium and silicon clusters as case studies
14:10-14:45	TOBIAS LAU (HZB, Germany) Valence electron delocalization and quenching of the local magnetic moment in mono and dibenzene complexes of Cr <sup>+</sup> and Mn <sup>+</sup>
14:45-15:25	LAI-SHENG WANG (Brown University, USA) Probing the electronic structure and chemical bonding of size-selected boron and doped-boron clusters using photoelectron spectroscopy
Coffee break	15:25-16:00
16:00-16:35	OTTO DOPFER (TU Berlin, Germany) Structures of silicon ions and clusters: silane ions and doping on the nanoscale
16:35-17:10	CHIARA PANOSSETTI (TU München, Germany) Better (random) walking through chemistry: how not to get lost in vast configurational spaces
17:10-17:50	THOMAS FRAUENHEIM (University of Bremen, Germany) DFTB <sup>+</sup> - An approximate DFT method: Applications to ground and excited state simulations of nanomaterials
Free Evening	

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Thursday, February 23<sup>rd</sup>

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9:00-9:40	HANNU HÄKKINEN (University of Jyväskylä, Finland) Towards controlled assemblies of ligand-stabilized noble metal nanoclusters
9:40-10:15	ANDRÉ FIELICKE (TU Berlin, Germany) High resolution anion photoelectron spectroscopy of the platinum trimer
10:15-10:55	TATSUDYA TSUKUDA (University of Tokyo, Japan) Gold superatoms and superatomic molecules protected by ligands

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Coffee break	10:55-11:25
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11:25-12:00	MARIO DÄHNE (TU Berlin, Germany) Atomic and electronic structure of clusters on the Si(111)7x7 surface
12:00-12:40	ALEXANDER SARANIN (FEFU, IACP, Vladivostok, Russia) Metallic 2D alloys and compounds on Si(111) and Ge(111) surfaces

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Lunch	12:40-14:00
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14:00-14:35	PETER R. SCHREINER (Universität Giessen, Germany) Nanodiamondoid physics through the eyes of a chemist
14:35-15:15	ÁDÁM GALI (Hungarian Academy of Sciences, Hungary) Ab-initio theory on doped diamond, silicon and silicon carbide nanoclusters
15:15-15:50	TORBJÖRN RANDE (TU Berlin, Germany) UV absorption of diamondoid - metal cluster hybrid systems

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Coffee break	15:50-16:20
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16:20-17:00	HORST WELLER (Universität Hamburg, Germany) Dynamics of semiconductor nanocrystal formation and their use in technical and biomedical applications
17:00-17:40	NORI SHINOHARA (Nagoya University, Japan) Putting diamondoids and diamondoid-nanowires into carbon nanotubes

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Conference dinner "Allegretto A Tavola"	19:00
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Friday, February 24<sup>th</sup>

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9:00-9:40 RICHARD PALMER (Taylor and Francis Group, UK)  
Atomic structure and mass-production of size-selected clusters

9:40-10:15 ROLAND MITRIC (Universität Würzburg, Germany)  
Theoretical modelling of light induced functionality in clusters, molecular aggregates and metal-organic hybrids

10:15-10:55 FRANCESCA BALETTO (King`s College London, UK)  
Numerical modelling for a rational design of metallic nanoparticles

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Coffee break 10:55-11:25

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11:25-12:00 CHRISTOPH TYBORSKI (TU Berlin, Germany)  
Raman spectroscopy of  $sp^2$  and  $sp^3$  carbon systems

12:00-12:35 PETER SAALFRANK (Universität Potsdam, Germany)  
Correlation function approach to radiative and non-radiative vibronic transitions in molecular systems

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Closing remarks

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