



SFB 1083

Structure and Dynamics
of Internal Interfaces

Kick-Off Meeting

Philipps-Universität Marburg

November 27 – 29, 2013



Foto: Peter Müller

Scientific Program

Wednesday, 27 November 2013

Welcome and Introduction (Renthof 5, GrHs)

13:30 – 13:50 **Ulrich Höfer**
Structure and Dynamics of Internal Interfaces - Overview

Inorganic Interfaces I (Chair: Hrvoje Petek)

13:50 – 14:20 **Stephan W. Koch**
Type-II excitons at semiconductor interfaces – introduction and theory

14:20 – 14:40 **Wolfgang Stolz**
MOVPE of semiconductor heterointerfaces and laser structures

14:40 – 15:00 **Arash Rahimi-Iman**
THz spectroscopy of semiconductor interfaces

15:00 – 15:30 Coffee Break

Inorganic Interfaces II (Chair: Martin Koch)

15:30 – 16:00 **Kerstin Volz**
Atomic scale structural characterization of the GaP/Si(001) interface

16:00 – 16:20 **Kristina Brixius**
Optical second harmonic generation of GaP/Si

16:20 – 16:50 **Kunie Ishioka**
Coherent phonons at the GaP/Si interface

Poster Session

17:00 – 20:00 Renthof 5, Foyer

Thursday, 28 November 2013

09:15 – 12:30 Discussion Meetings / Topical Workshops
(Renthof 5, SR LBII, SR Didaktik, Rm. 01002, 01009)

Organic/Metal Interfaces (Chair: Gregor Witte)

- 13:30 – 14:00 **Michael Gottfried**
Reactive metal/organic interfaces: Metals on semiconducting polymers and surface-assisted organic synthesis
- 14:00 – 14:20 **Ilya Nechaev**
DFT investigation of organic/metal interface states
- 14:20 – 14:40 **Andreas Namgalies**
Carrier dynamics at the PTCDA/Ag(111) interface
- 14:40 – 15:00 **Peter Jakob**
Vibrational spectroscopy of CuPc/PTCDA bilayer systems
- 15:00 – 15:30 Coffee Break

Organic/Organic Interfaces (Chair: Daniel Sánchez-Portal)

- 15:30 – 15:50 **Tobias Breuer**
Investigation of pentacene/C₆₀ interfaces: diffusion-controlled growth of two-, one-, and zero-dimensional C₆₀-nano-structures
- 15:50 – 16:10 **Sangam Chatterjee**
Dynamics of charge transfer at C₆₀ interfaces
- 16:10 – 16:30 **Katharina Gries**
Characterization of co-deposited pentacene/perfluoropentacene thin-films via transmission electron microscopy
- 16:30 – 16:50 **Martin Liebold**
Phthalocyanines with equatorial and axial anchors for organic interfaces with tailored properties
- 17:00 – 18:00 (Business meeting of the managing board)

Conference Dinner

19:00 – 23:00 Landgrafenschloss, Fürstensaal

Friday, 29 November 2013

Organic/Inorganic Semiconductor Interfaces I (Chair: Kerstin Volz)

- 09:15 – 09:35 **Michael Dürr**
Chemoselective attachment of organic molecules to silicon
- 09:35 – 09:50 **Gerson Mette**
Adsorption of cyclooctyne on Si(100)
- 09:50 – 10:10 **Ralf Tonner**
Density functional study of cyclooctyne adsorption on Si(100) and comparison to STM results
- 10:10 – 10:30 **Ulrich Koert**
Molecular building blocks for functional organic interfaces
- 10:30 – 11:00 Coffee Break

Organic/Inorganic Semiconductor Interfaces II (Chair: Jörg Sundermeyer)

- 11:00 – 11:20 **Stefanie Dehnen**
Molecular inorganic/organic/inorganic multilayer clusters
- 11:30 – 11:50 **Gregor Witte**
Preparation of organic/inorganic semiconductor interfaces with predefined molecular orientation
- 11:50 – 12:10 **Wolfram Heimbrod**
Optical studies of organic-inorganic hybrid semiconductors
- 12:10 – 12:30 **Peter Koval**
Using basis sets of local functions for efficient TDDFT and GW calculations

Résumé, Discussion and Meeting of Members (Chair: Ulrich Höfer)

- 12:30 – 13:00 *Election of a students' representative*
Overview of future SFB activities
Teaching program of GRK 1782 "Functionalization of Semiconductors"

List of Posters

Renthof 5, 1st Floor

(A1) Philip Hens, **Wolfgang Stolz**

Metal Organic Vapour Phase Epitaxy of Semiconductor Heterostructures and Interfaces

(A2) Tobias Breuer, Andrea Karthäuser, Michael Klues, Michael Kothe, Alexander Mänz, **Gregor Witte**

Inorganic/Organic and Organic/Organic Interfaces: Structure and Charge Transport

(A3) Carolin Braatz, **Peter Jakob**, Gregor Öhl, Sabastian Thussing

Organic Heterolayer Interfaces: Structure and Vibrational Excitations

(A4) Min Chen, Hans-Jörg Drescher, **Michael Gottfried**, Benedikt Klein, Han Zhou, Malte Zugermeier

Reactivity, Energetics and Structure of Buried Organic/Metal Interfaces

(A5) Andreas Beyer, María del Rocío Félix Ángel, **Katharina Gries**, Han Han, Jandieri Kakhaber, **Kerstin Volz**

Atomically Resolved Structure of Solid/Solid Interfaces

(B7) Benjamin Breddermann, **Stephan W. Koch**, Christoph Möller, **Wolfgang Stolz**

Interface-Dominated Semiconductor Laser Structures

Renthof 5, 2nd Floor

(A7) Eduard Baal, Malcolm Bartlett, Ahmed Bayoumi, Martin Liebold,

Jörg Sundermeyer

Functional Design and Synthesis of Metal Organic Chromophores for Heterojunction Interfaces

(A8) Ruben Bartholomäus, **Ulrich Koert**, Niels Münster, Jonas Schwaben

Organic Molecular Building Blocks for the Synthesis of Internal Interfaces

(A9) **Stefanie Dehnen**, Eliza Leusmann, Matthias Reinmuth, Niklas Rinn, Zhilian You

Synthesis and Properties of Molecular Inorganic/Organic/Inorganic Multilayer Clusters

(Ö) **Stefanie Dehnen**, **Heinz Jänsch**, Bastian Weinert

Public Relations Project

List of Posters (continued)

Renthof 5, 3rd Floor

(A6) Josua Pecher, Marc Raupach, **Ralf Tonner**

Unified Density Functional Description of Bonding and Interactions at Inorganic/Organic Interfaces

(B1) Sebastian Gies, **Wolfram Heimbrodt**, Uwe Kaiser, Carsten Kruska, Ingo Meyenburg

Optical Spectroscopy at Internal Interfaces – Semiconductor Heterostructures and Organic-Inorganic Hybrids

(B2) **Sangam Chatterjee**, Robin Döring, Kolja Kolata, Jan Kuhnert, Andre Rinn, Nils Rosemann

Ultrafast Spectroscopy and Control of Excitations Across Internal Interfaces

(B3) Michael Drexler, **Martin Koch**, Arash Rahini-Iman

THz- and Time-Resolved Optical Spectroscopy on Buried Interfaces

(B4) Christian Berger, Christoph Böttge, Dominik Breddermann, **Mackillo Kira**, **Stephan W. Koch**, Phillip Springer, Osmo Vänskä

Microscopic Theory of Optical Excitations in Interface-Dominated Material Systems

(B5) Kristina Brixius, Michael Dürr, Jens Güdde, **Ulrich Höfer**, Alexander Lerch, Gerson Mette

Time-Resolved Nonlinear Optical Spectroscopy at Buried Semiconductor Interfaces

(B6) Nico Armbrust, **Ulrich Höfer**, Andreas Namgalies, Dennis Noll, Jonas Zimmermann

Time-Resolved Two-Photon Photoemission Studies of Interface Electron and Exciton Dynamics

(GP1) Eugene V. Chulkov, **Pedro M. Echenique**, Thomas Frederiksen, Peter Koval, Frederico Marchensin, Ilya Nechaev, **Daniel Sánchez-Portal**, Stepan Tsirkin, Nikolay Zaitsev

Electron Dynamics at Organic/Inorganic Interfaces from First Principles

Overview

	Wednesday	Thursday	Friday	
09:15		Discussion Meetings Topical Workshops <i>(Renthof 5, SR LBII, SR Didaktik, Rm. 01002, 01009)</i>	Org./Inorg. Semiconductor Interfaces I Michael Dürr Gerson Mette Ralf Tonner Ulrich Koert	
09:30				Coffee Break
09:45				Org./Inorg. Semiconductor Interfaces II Stefanie Dehnen Gregor Witte Wolfram Heimbrod Peter Koval
10:00				
10:15				
10:30				
10:45				
11:00				
11:15				Résumé, Discussion and Meeting of Members Ulrich Höfer / Kerstin Volz
11:45				
12:00				
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13:45	Inorganic Interfaces I			
14:00	Stephan W. Koch			
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14:30	Arash Rahimi-Iman			
14:45				
15:00	Coffee Break	Coffee Break		
15:15				
15:30	Inorganic Interfaces II	Organic/Organic Interfaces Tobias Breuer Sangam Chatterjee Katharina Gries Martin Liebold		
15:45	Kerstin Volz			
16:00	Kristina Brixius			
16:15	Kunie Ishioka			
16:30				
16:45				
17:00	Poster Session <i>Renthof 5, Foyer</i>	Business meeting of the managing board		
17:15				
17:30				
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18:00				
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19:00			Conference Dinner <i>Landgrafenschloss, Fürstensaal</i>	
19:15				
19:30				
19:45				

Collaborative Research Centre SFB 1083

Established at Philipps-Universität Marburg in collaboration with the Donostia International Physics Center (DIPC), San Sebastián, Spain, the SFB consists of more than 60 chemists and physicists that collaborate in investigations of solid/solid interfaces of a variety of organic and inorganic materials. The aim is to achieve a detailed microscopic understanding of the chemical bonding, the electronic coupling, and the dynamics of energy transfer for model systems of different classes of hetero-interfaces.

Principle Investigators

PD Dr. Sangam Chatterjee	Department of Physics
Prof. Dr. Stefanie Dehnen	Department of Chemistry
Prof. Dr. Pedro M. Echenique	DIPC, San Sebastián, Spain
Prof. Dr. Michael Gottfried	Department of Chemistry
Dr. Katharina Ines Gries	Department of Physics and WZMW
Prof. Dr. Wolfram Heimbrod	Department of Physics
Prof. Dr. Ulrich Höfer	Department of Physics
Prof. Dr. Peter Jakob	Department of Physics
Prof. Dr. Heinz J. Jänsch	Department of Physics
Prof. Dr. Mackillo Kira	Department of Physics
Prof. Dr. Martin Koch	Department of Physics
Prof. Dr. Stephan W. Koch	Department of Physics
Prof. Dr. Ulrich Koert	Department of Chemistry
Dr. Daniel Sánchez-Portal	DIPC, San Sebastián, Spain
Dr. Wolfgang Stolz	Material Sciences Center (WZMW)
Prof. Dr. Jörg Sundermeyer	Department of Chemistry
Dr. Ralf Tonner	Department of Chemistry
Prof. Dr. Kerstin Volz	Department of Physics and WZMW
Prof. Dr. Gregor Witte	Department of Physics

Associated Members

Prof. Dr. Michael Dürr	Institute of Applied Physics, Gießen
Prof. Dr. Gerhard Hilt	Department of Chemistry, Marburg
Dr. Kunie Ishioka	National Institute for Materials Science, Tsukuba, Japan
Prof. Dr. Hrvoje Petek	Department of Physics, University of Pittsburgh, USA