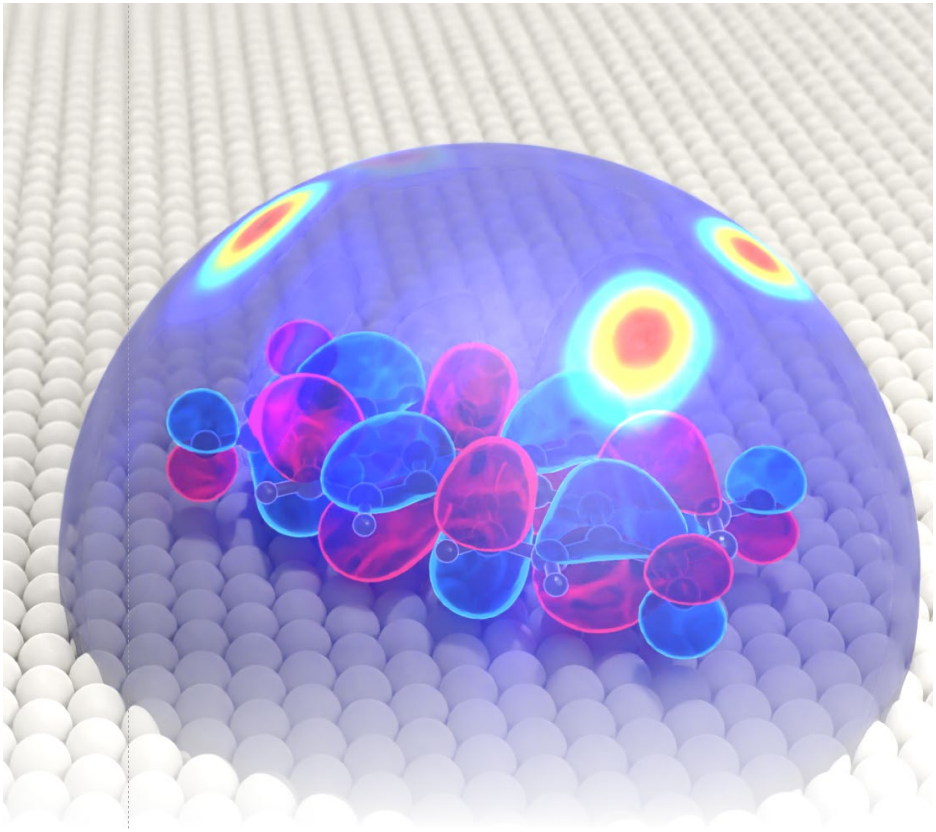
SFB 1083 Workshop
Organic Interfaces and Orbital Tomography



Philipps-Universität Marburg

Lecture Hall, Renthof 5
March 6-7, 2023

Scientific Program

SFB 1083
Structure and Dynamics
of Internal Interfaces

Philipps Universität Marburg

Collaborative Research Centre 1083
Structure and Dynamics of Internal Interfaces
Philipps-Universität Marburg
Prof. Dr. Kerstin Volz (spokesperson)

Dr. Stefan R. Kachel (SFB 1083 office)

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The structure and dynamics of well-defined organic donor/acceptor interfaces, as well as of interfaces between ordered organic layers and single crystal inorganic substrates, play a central role in SFB 1083 [1]. Photoemission orbital tomography has unique capabilities to determine the electronic properties of such interfaces at the molecular orbital level [2]. Moreover, its extension to the time-domain allows investigations of transiently excited molecules [3].

The latter development and the demonstration of subcycle time-resolution in angle resolved photoemission [4] form the basis of “Orbital Cinema”, a new synergy project funded by the European Research Council (ERC) that aims at coherent driving, actively shaping, and functionalizing orbitals with light waves [5].

SFB 1083 and Orbital Cinema have different scientific scopes, yet they work with similar model systems and rely on related experimental and theoretical methods. The aim of this workshop is to bring scientists of SFB 1083 and Orbital Cinema together in order to discuss common interests and to explore the potential for future collaboration.

[1] www.internal-interfaces.de
[2] en.wikipedia.org/wiki/Photoemission_orbital_tomography
[3] Wallauer *et al.*, Science **371**, 1056 (2021) DOI: 10.1126/science.abf3286
[4] Reimann *et al.*, Nature **562**, 396 (2018) DOI: 10.1038/s41586-018-0544-x
[5] www.orbital-cinema.eu

Monday, 6 March 2023

13:15 – 14:00 Arrival & Lunch

14:00 – 14:10 **Ulrich Höfer**
Welcome & Introduction to SFB 1083 and ERC Orbital Cinema

Session I (Chair: Rupert Huber)

14:10 – 14:40 **Stefan Tautz** (Jülich)
Recent developments in photoemission orbital tomography

14:40 – 15:00 **Josef Freudenstein** (Regensburg)
Attoclocking Bloch electrons in atomically thin solids

15:00 – 15:20 **Joshua Thompson** (Marburg, AG Malic)
Exciton optics and dynamics at organic/TMDC interfaces

15:20 – 15:50 **Peter Puschnig** (Graz)
Photoemission orbital tomography for optically excited states

15:50 – 16:20 Coffee Break

Session II (Chair: Jens Güdde)

16.20 – 16:40 **Pierre Dombrowski** (Marburg, AG Witte)
Shape control in organic nanostructures on TMDC surfaces

16:40 – 17:00 **Suguru Ito** (Marburg, AG Höfer)
Lightwave ARPES – buildup and dephasing of Floquet-Bloch bands on subcycle time scales

17:00 – 17:20 **Robert Wallauer** (Marburg)
Time-resolved momentum microscopy – basic principles and considerations for lightwave ARPES

17:20 – 17:40 **Christian Kern** (Graz)
Photoemission angular distributions from time-dependent density functional theory

17:40 – 19:20 **Session III - Posters**

20:00 Dinner

Tuesday, 7 March 2023

08:30 – 10:00 **Session IV – Posters & Labtour AG Höfer**

Session V (Chair: Ulrich Koert**)**

10:00 – 10:30 **Michael Gottfried** (Marburg)
On-surface synthesis of atomically thin carbon materials

10:30 – 10:50 **Ulrich Höfer, Rupert Huber** (Marburg/Regensburg)
Orbital tomography of lightwave-driven molecular systems at the Regensburg Center for Ultrafast Nanoscopy (RUN)

10:50 – 11:20 Coffee break

Session VI (Chair: Christian Kumpf)

11:20 – 11:40 **François Bocquet** (Jülich)
Dedicated organic systems for orbital tomography

11:40 – 12:00 **Peter Jakob** (Marburg)
Vibrational frequency as internal clock for timing molecule-metal charge transfer

12:00 – 12:20 **Carmen Roelcke** (Regensburg)
Orbital videography and control of a dancing molecule on a surface

12:20 – 14.00 **Session VII – Posters**
Lunch

14:00 Departure

Posters

1) **Alexa Adamkiewicz, Marcel Theilen** (Marburg, AG Höfer)
Time-resolved photoemission orbital tomography of CuPc on Cu(001)-2O

2) **Michael Aschenbrenner, Jakob Helml, Manuel Meierhofer** (Regensburg)
Attosecond stabilization of phase-locked multi-THz waveforms

3) **Dominik Brandstetter** (Graz)
Real-time pump-probe simulations within time-dependent density functional theory

4) **Timo Glaser, Michael Dürr** (Gießen), **Dominik Scharf** (Marburg,AG Koert)
Towards π-wires on a semiconductor surface: Benzyne on Si(001)

5) **Darius Günder** (Marburg, AG Witte)
F-center-mediated growth of patterned organic semiconductor films on alkali halides

6) **Jan Herritsch** (Marburg, AG Gottfried)
On-surface reactions of a Lead-Porphyrin on Au(111) and Cu(111)

7) **Christian Kumpf** (Jülich)
hBN on metals as template for organic layers

8) **Manuel Meierhofer, Vincent Eggers, Jakob Helml** (Regensburg)
Next-generation high-field multi-terahertz source for lightwave ARPES

9) **Florian Münster, Leonard Neuhaus** (Marburg, AG Gottfried)
On-surface Porphyrin metalation with Cesium

10) **Lasse Münster** (Marburg, AG Höfer)
Imaging of valley population in monolayer WS_2

11) **Dominik Muth** (Marburg, AG Gerhard)
Comparison of exciton diffusion in organic and inorganic semiconductors

12) **Tim Naumann** (Marburg, AG Gottfried)
On-surface synthesis of Kekulene and Isokekulene

13) **Ravi Priya, Weishan Wu** (Marburg, AG Jakob)
Long range ordering of molecular layers

14) **Daniel Riese, Manuel Meierhofer** (Regensburg)
Non-integer high-harmonic generation in topologically protected surfaces

15) **Carmen Roelcke, Rupert Huber** (Regensburg)
Nanovideography of ultrafast charge transfer across an atomic-scale interface

16) **Serguei Soubatch** (Jülich)
Measuring molecular distortion and hybridization with orbital tomography

17) **Klaus Stallberg** (Marburg, AG Höfer / Clausthal)
Interface-state mediated charge transfer at organic/metal interfaces

18) **Monja Stettner** (Jülich)
Design of sample systems for the investigation of interlayer excitons

19) **Joshua Thompson, Samuel Brem, Roberto Rosati** (Marburg, AG Malic)
Exciton optics, dynamics and transport in atomically thin materials

20) **Sarah Zajusch, Suguru Ito** (Marburg, AG Höfer)
Analysis of multidimensional photoemission data – correction of symmetry distortion and photoelectron streaking

List of Participants

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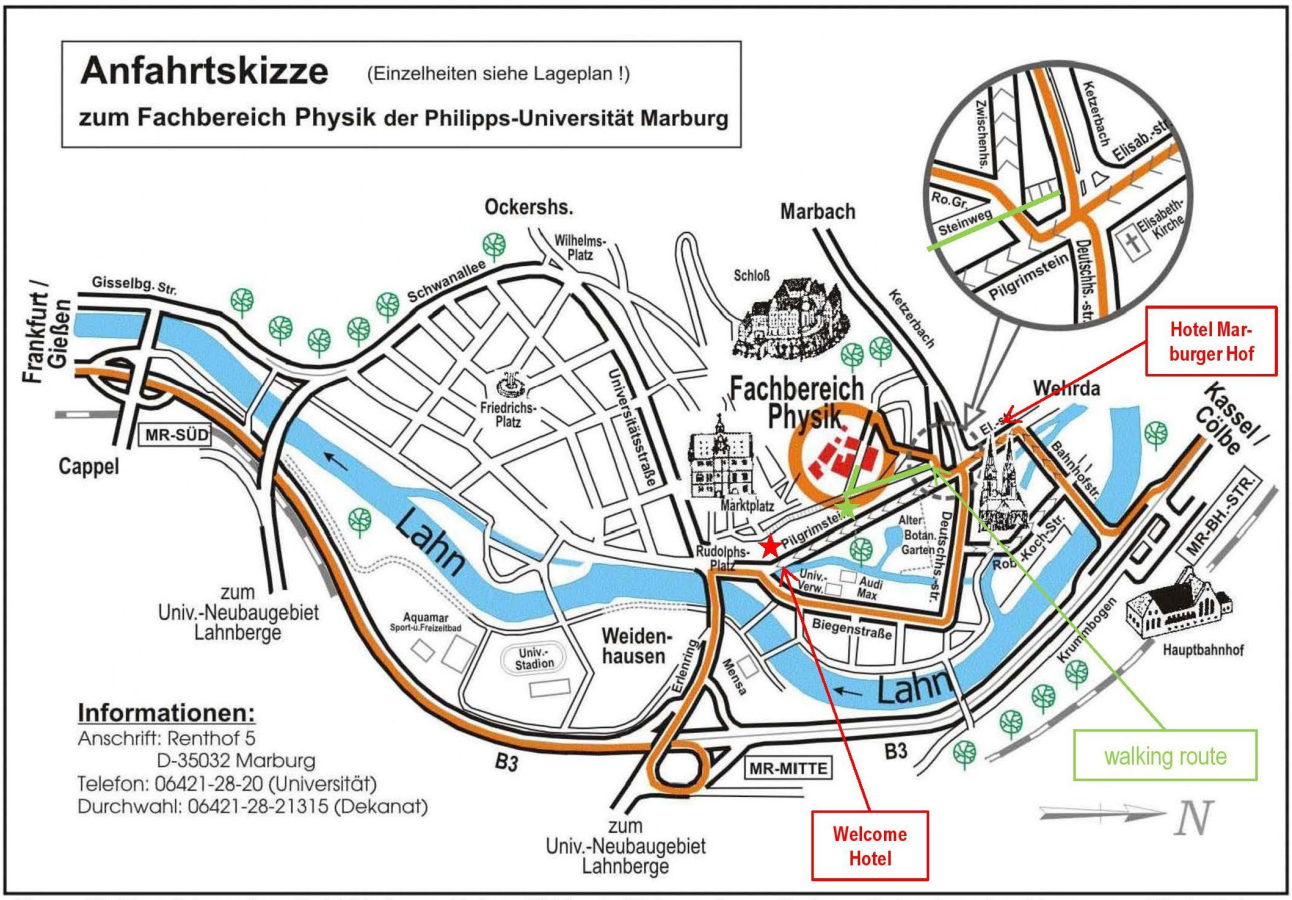

Above: Walking distance from Hotel Marburger Hof ca. 10 Min via Steinweg (green line) or a 2 elevators at parking garage Pilgrimstein (green star). The Welcome Hotel is situated right across from elevators/stairs (red star) up to the Oberstadt.

Below: Access Renthof 5 to the right of the blue star. Offices Prof. Höfer (spokesman SFB 1083) and SFB-office on 1st floor.