

RTG PCL Summer School 2024 at NH Prague City, Mozartova 261/1, 15000 Prague | PROGRAM


Time	Monday Sep 23	Tuesday Sep 24	Wednesday Sep 25	Thursday Sep 26	Friday Sep 27	
09:00 - 09:30		Lecture 3: Pascal Ruffieux (EMPA)	<i>Mounting of posters 9-15</i>	Complementary skills session (1.5 h)	Open Book session 2 (2 h)	
09:30 - 10:00			GA meeting (1 h)			
10:00 - 10:30		Coffee break (30 min)				
10:30 - 11:00		Visit to the Nanosurf Lab (Jelinek)		Coffee break (30 min)	Coffee break (30 min)	
11:00 - 11:30				Open Book session 1 (1.5 h)	Complementary skills session (1.5 h)	Coffee break (30 min)
11:30 - 12:00						Poster award & Closing (30 min)
12:00 - 12:30						Farewell lunch (hotel)
12:30 - 13:00					Lunch (hotel)	Lunch (hotel)
13:00 - 13:30			Lunch (hotel), Welcome coffee & Registration	Lunch (hotel)	Poster flash presentations 2 (30 min)	Complementary skills session (2 h)
13:30 - 14:00		Poster session 2 (1.5 h)				
14:00 - 14:30	<i>Mounting of posters 1-8</i>					
14:30 - 15:00	Poster flash presentations 1 (30 min)					
15:00 - 15:30	Opening remarks (30 min, may be shorter)	Poster session 1 (1 h)				
15:30 - 16:00	Lecture 1: Pavel Jelinek (CAS)	Coffee break (30 min)	Coffee break (30 min)	Coffee break (30 min)		
16:00 - 16:30	Coffee break (1 h)	Poster session 1 (1.5 h)	Poster session 2 (1 h)	Complementary skills session (1.5 h)		
16:30 - 17:00						
17:00 - 17:30						
17:30 - 18:00	Lecture 2: Otakar Frank (CAS)		Social activity			
18:00 - 18:30						
18:30 - 19:00						
19:00 - 20:30	Dinner (hotel)					

Monday, September 23

Time	Activity	Speaker
13:00 – 15:00	<i>Lunch (hotel), Welcome coffee & Registration</i>	
15:00 – 15:30	Opening	Prof. Thomas Heine
15:30 - 16:30	L1: Origin of π-magnetism in polyaromatic hydrocarbons	Dr. Pavel Jelinek
16:30 - 17:30	<i>Coffee break</i>	
17:30 - 18:30	L2: (Nano)spectroscopic signatures of intricate relations between 2D layers and their substrate	Dr. Otakar Frank
19:00	<i>Dinner (hotel)</i>	

Tuesday, September 24

Time	Activity	Speaker
09:00 – 10:00	L3: On-surface Synthesis of Graphene Nanoribbons and Spin Chains	Dr. Pascal Ruffieux
10:00 – 10:30	<i>Coffee break</i>	
10:30 – 13:00	Visit to the Nanosurf Lab (Dr. Pavel Jelinek)	
13:00 – 14:00	<i>Lunch (hotel)</i>	
14:00 – 14:30	<i>Mounting of posters 1-8</i>	Doctoral Researchers
14:30 – 15:00	Poster flash presentations 1 (Posters 1-8)	Doctoral Researchers
15:00 – 16:00	Poster session 1 (Posters 1-8)	Doctoral Researchers
16:00 – 16:30	<i>Coffee break</i>	
16:30 – 18:00	Poster session 1 (Posters 1-8)	Doctoral Researchers

 **Nanosurf Lab:** Cukrovarnická 10, 162 00 Prague 6

Wednesday, September 25

Time	Activity	Speaker
09:00 – 9:30	<i>Mounting of posters 9-15</i>	Doctoral Researchers
9:30 – 10:30	GA meeting	GA members
10:30 – 11:00	<i>Coffee break</i>	
11:00 – 12:30	Open Book session 1	All
12:30 – 13:30	<i>Lunch (hotel)</i>	
13:30 – 14:00	Poster flash presentations 2 (Posters 9-15)	Doctoral Researchers
14:00 – 15:30	Poster session 2 (Posters 9-15)	Doctoral Researchers
15:30 – 16:00	<i>Coffee break</i>	
16:00 – 17:00	Poster session 2 (Posters 9-15)	Doctoral Researchers
17:00 – 17:30		
17:30 – 20:30	Social activity	

Thursday, September 26

Time	Activity	Speaker
09:00 – 10:30	“Conflict management throughout the doctorate: From squabbles to a culture of conflict” (Session 1)	Robert Pfeiffer
10:30 – 11:00	<i>Coffee break</i>	
11:00 – 12:30	“Conflict management throughout the doctorate: From squabbles to a culture of conflict” (Session 2)	Robert Pfeiffer
12:30 – 13:30	<i>Lunch (hotel)</i>	
13:30 – 15:30	“Conflict management throughout the doctorate: From squabbles to a culture of conflict” (Session 3)	Robert Pfeiffer
15:30 – 16:00	<i>Coffee break</i>	
16:00 – 17:30	“Conflict management throughout the doctorate: From squabbles to a culture of conflict” (Session 4)	Robert Pfeiffer

Friday, September 27th

Time	Activity	Speaker
09:00 – 11:00	Open Book session 2	All
11:00 – 11:30	<i>Coffee break</i>	
11:30 – 12:00	Poster award & Closing	
12:00 – 13:00	<i>Farewell Lunch (hotel)</i>	

Oral contributions, Sep 23 -24

Invited Speaker	Title of presentation
Dr. Pavel Jelinek	Origin of π-magnetism in polyaromatic hydrocarbons
Dr. Otakar Frank	(Nano)spectroscopic signatures of intricate relations between 2D layers and their substrate
Dr. Pascal Ruffieux	On-surface Synthesis of Graphene Nanoribbons and Spin Chains

Invited Speakers: Talk abstracts and short bio

L1: Origin of π -magnetism in polyaromatic hydrocarbons

Dr. Pavel Jelinek

Institute of Physics of the Czech Academy of Sciences, Prague

The recent progress in on-surface synthesis enabled the formation of new molecular structures, which are unavailable in traditional organic chemistry in solution [1]. Special attention was paid to the on-surface synthesis of open-shell polyaromatic hydrocarbons (PAH), which showed interesting magnetic properties [2].

In this talk, we will provide a brief review of different strategies to introduce π -magnetism in PAHs, including the frustrated topology of bipartite lattice or electron-electron correlation [3]. We will present a synthesis of polyradical molecules with a strong multireference character. Their electronic structure is analyzed using the SPM technique, including nickelocene functionalized probes and many-body CAS calculations, enabling us to describe the strongly correlated multireference states [5] properly. We will discuss a PAH molecule, where a combination of the e-e interaction and the frustrated topology introduces a strongly entangled tetraradical character.

We will also discuss the connection between the topological band structure of π -conjugated polymer introduced in the framework of the Su-Schrieffer-Heeger (SSH) model and their π -conjugation form. We will discuss the quantum phase transition between two topologically distinct phases in an π -conjugated polymer [3]. This quantum phase transition is defined by the length of the polymer, triggered by the transition from topologically trivial to a non-trivial phase above a certain polymer length. We demonstrate that the pseudo Jahn-Teller effect is the driving mechanism responsible for the quantum phase transition [4].

References

[1] S. Clair and D. G. de Oteyza, *Chemical Reviews* **119**, 4717 (2019).

- [2] J. Li et al., Nature Communication **10**, 200 (2019); N. Pavlicek et al., Nature Nanotechnology **12**, 308 (2017); S. Mishra et al., Nature Nanotechnology **15**, 22 (2019); O. Gröning, et al., Nature **560**, 209 (2018); D.J. Rizzo, et al., Nature **560**, 204 (2018)
- [3] R. Ortiz et al., Nano Letters **19**, 5991 (2019).
- [4] S. Song et al. Nature Chem **16**, 938 (2024).
- [5] B. Cierra et al, Nature Nano, **15**, 437 (2020).
- [6] H. Gonzalez-Herrero et al, Adv. Mat. **33**, 2104495 (2021).

Short Bio: Pavel Jelinek is a senior researcher at the Institute of Physics of the Czech Academy of Sciences. He founded the research NANOSURF group, which strongly benefits from the synergy between experiment and theory. His research field is on surface synthesis, molecular electronics, low dimensional materials, scanning probe microscopy, and strongly correlated systems. He received several national research awards, including Praemium Academiae (Czech Academy of Sciences) and The Rudolf Lukes Prize (Czech Chemical Society).

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L2: (Nano)spectroscopic signatures of intricate relations between 2D layers and their substrate

Dr. Otakar Frank

J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Dolejškova 2155/3, 182 23 Prague

Common spectroscopic investigation of two-dimensional materials and their van der Waals (vdW) heterostructures mostly relies either on diffraction-limited micro-Raman or photoluminescence (PL). However, these methods do not properly capture local variations caused by, *e.g.*, nanometre-sized heterogeneities stemming from contamination trapped between the layers or complex strain and charge patterns formed by strong out-of-plane interactions.

Tip-enhanced spectroscopy methods enable access to information on the local lattice deformation and also on the interaction between the individual layers composing the heterostructure. What may appear as peak splitting in micro-Raman or PL spectra of transition metal dichalcogenides (TMDC) on metal substrates or of vdW heterobilayers, can, in fact, often come from mixing up signals from various regions within the laser spot, including new or discretely shifted peaks. In other cases, however, peak splitting can indicate lifting the degeneracy of the phonon, due to, for example, uniaxial deformation. Spectroscopic fingerprints, both on micro- and nanoscale, of variously interacting vdW layers will be discussed, including TMDCs on metals [1-3] and TMDC heterobilayers [4-6].

References:

- [1] Velicky et al. J. Phys. Chem. Lett. **11**, 6112 (2020);
- [2] Velicky et al. Adv. Mater. Interfaces **7**, 2001324 (2020);
- [3] Rodriguez et al. Phys. Rev. B **105**, 195413 (2022);
- [4] Rodriguez et al. 2D Mater. **8**, 025028 (2021);
- [5] Rodriguez et al. J. Phys. Chem. Lett. **13**, 5854 (2022);
- [6] Rodriguez et al., ACS Nano **17**, 7787 (2023)

Short Bio: Dr. Otakar Frank is a senior researcher and the Head of the Department of Electrochemical Materials at J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences in Prague, Czech Republic. He obtained his Ph.D. degree in 2005 at the Charles University in Prague. Before rejoining his current position, he spent two years as a post-doctoral fellow at the Institute of Chemical Engineering in Patras, Greece, and several shorter stays, *e.g.*, at MIT, Argonne National Laboratory, IFW Dresden, etc. His research is focused mainly on the mechanical, electronic, and electrochemical properties of graphene and related nanostructures, using various micro- and nano- in-situ spectroscopic methods.

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L3: On-surface Synthesis of Graphene Nanoribbons and Spin Chains

Dr. Pascal Ruffieux

Swiss Federal Laboratories for Materials Science and Technology (Empa), Dübendorf

Recent advances in on-surface synthesis has allowed the selective fabrication of a number of prototypical types of graphene nanoribbons. The thereby achieved properties include width-dependent electronic band gaps in armchair graphene nanoribbons, edge-localized states in zigzag graphene nanoribbons and topological band engineering in width-modulated topological graphene nanoribbons. Here, I will discuss some important properties, their synthesis and device integration of armchair graphene nanoribbons.

More recently, on-surface synthesis of magnetic nanographenes has been reported. Here, the spin originates from unpaired electrons present in nanographenes with controlled sublattice imbalance or topological frustration. The corresponding magnetic moments live in π -orbitals and are hence largely delocalized, which allows for chemical control over their exchange interaction when covalently linking molecular building blocks. Here, I will present synthesis of various prototypical magnetic nanographenes and the possibility to covalently link them to form coupled spin systems where exchange coupling can exceed 100 meV. Using halogen-substituted precursors, we achieve the on-surface synthesis-based deterministic bottom-up fabrication of various spin chains including a triangulene spin-1 chain revealing the predicted Haldane gap and fractional excitations at the chain termini or a strictly alternating spin- $\frac{1}{2}$ chain with chemically engineered coupling strengths J_1 and J_2 . Scanning tunneling microscopy and spectroscopy is used to explore length- and site-dependent magnetic excitations. Furthermore, we apply hydrogenation to achieve spin site passivation and controlled tip-based local reactivation to fabricate and characterize specific spin patterns in one-dimensional spin chains and spin clusters.

Short Bio: Pascal Ruffieux received his PhD in 2002 at the University of Fribourg (Switzerland) and joined the Laboratories for Materials Science and Technology (Empa) in 2003. As Group Leader of the Carbon Nanomaterials Research Group he is focusing on the on-surface synthesis of atomically-defined carbon nanostructures and their electronic and magnetic characterization. He has a strong background in scanning probe microscopy and spectroscopy (STM and STS) as well as photoelectron spectroscopy (ARPES, XPS, XPD). He received several awards such as the Charmey Prize of the SAOG and the Empa Research Prize and is currently board member of the Swiss Physical Society. He has given numerous invited talks at international conferences and has published more than 100 peer-reviewed papers.

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Poster contributions, Sep 24 -25

Nr.	Doctoral Researchers (PI groups)	Poster Titles for session on Sep 24
1	Boris Borisov (A2, Feng)	Precision Synthesis of Saddle Nanographene and Graphene Nanoribbons with edge helicity
2	Kevin Gerein (A3, Hirsch)	Modular Chemical Patterning of Graphene by Direct Laser Writing Using λ^3 -Iodanes
3	Aleena Jose (A4, Kaskel)	2,2' Diacetyl biphenyl as a precursor for porous graphitic carbon for electric double-layer capacitors
4	Majid Shaker (A5, Steinrück)	TBA
5	Jiwon Byun (B1, Halik)	Visible-light responsive photo-switching HTI (Hemithioindigo) SAMs on surface
6	Sijia Feng (B4, Weber)	Investigation of light-matter interaction under the environmental control of 2D materials via squeezable nanojunction technique
7	Jannis Kocklauener (C2, Golze)	Prediction of core-level satellites from highly accurate Green's function methods
8	Elena Mack (C3, Guldi)	Interfacial charge transfer states: a study in dispersion and solid state

Nr.	Doctoral Researchers (PI groups)	Poster Titles for session on Sep 25
9	Paul-Alexander Laval-Schmidt (A1, Dong)	2D conjugated metal-organic framework for quantum information science
10	Johanna Krüger (Associated, Hirsch, A)	Spatially resolved 2D Laser Writing of Graphene with Diazonium Salts
11	Tamara Nagel (Associated, Hirsch, A)	Towards Highly Controlled 2D-Engineering of Graphene
12	Giovanni Beneventi (Associated, Guldi, B,C)	Lateral π -extended molecular nanographene
13	Shreya Garg (B3, Maier)	On-surface synthesis and study of GNRs with defect lines
14	Anjana Aravind (C1, Brunner)	Processing Chitin-Graphene Oxide into Stable Composite Materials for Efficient Heavy Metal Adsorption from Aqueous Solution
15	Linda Feuerstein (C5, Weidinger)	Local Electric Fields at Planar Carbon-based Electrodes

Poster 1

Precision Synthesis of Saddle Nanographene and Graphene Nanoribbons with edge helicity

*Boris Borisov**, Giovanni M. Beneventi, Yubin Fu, Zhen-lin Qiu, Hartmut Komber, Qing-song Deng, Phillip M. Greißel, Alejandro Cadrianel, Dirk Guldi, Ji Ma, Xinliang Feng

* Center for Advancing Electronics Dresden (cfaed) & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, Germany

Nonbenzenoid nanographenes (NGs), characterized by the incorporation of non-hexagonal rings, have garnered significant attention due to their unique topologies and exceptional physicochemical properties, positioning them as promising candidates for optoelectronic and spintronic applications. While pentagons induce positive curvature, heptagons and octagons generate concave, negatively curved structures. Among these, saddle-shaped NGs with heptagonal rings are pivotal for the development of three-dimensional carbon nanostructures such as schwarzite, which is predicted to exhibit remarkable electronic and magnetic properties. However, the synthesis of these NGs remains challenging due to the high-strain energies inherent in their highly twisted structures and the lack of efficient synthetic methods for heptagon incorporation.

Herein, a novel saddle-shaped nanographene (**1**) with four embedded heptagons is synthesized via a highly efficient Scholl reaction from a pre-designed oligophenylene precursor. Notably, a quadruple [6]helicene intermediate was also obtained and isolated by controlling the Scholl reaction conditions. Interestingly, single crystal structures of **1** display a saddle geometry induced by the four embedded heptagons, resulting in a deep curvature. Theoretical calculations at the molecular level suggest a weak antiaromatic character of the heptagons in **1**. Remarkably, compound **1** exhibits dual fluorescence from S_1 and S_2 . The deep-saddle-shaped geometry in **1** defines host-guest interactions with fullerenes, which were explored in titration experiments and by theoretical methods. The resulting **1**@ C_{60} are stable and are subject to an electron transfer from photoexcited **1** to C_{60} . Our current study underscores the influence of heptagon rings on the photophysical, self-assembly, and electron-donating properties of NGs.

In addition to the non-benzenoid NGs, curved GNRs (cGNRs) are gaining much attention these days. Capitalizing on their unconventional edge configurations, cGNRs demonstrably exhibit a significantly reduced band gap and superior charge carrier mobility compared to their planar counterparts of comparable widths. Furthermore, cGNRs possessing out-of-plane distortions present intriguing possibilities in the realms of nonlinear optics and asymmetric catalysis. However, the synthetic landscape for cGNRs remains relatively unexplored due to robust synthetic methodologies and the challenge of designing suitable molecular precursors.

The incursion of a [6]helicene subunit on the GNR periphery is the main object of this study. It is believed, that the presence of such an optically active fragment will induce structure with well-defined chirality, leading to the exploration of new optoelectronic or spintronic properties such as chirality induced spin-selectivity (CISS) effect.

References

- [1] Narita, A.; Feng, X.; Müllen, K. Bottom-Up Synthesis of Chemically Precise Graphene Nanoribbons: Bottom-Up Synthesis of Chemically Precise Graphene Nanoribbons. *Chem. Rec.* **2015**, *15* (1), 295–309. <https://doi.org/10.1002/tcr.201402082>.
- [2] Pun, S. H.; Miao, Q. Toward Negatively Curved Carbons. *Acc. Chem. Res.* **2018**, *51* (7), 1630–1642. <https://doi.org/10.1021/acs.accounts.8b00140>.
- [3] Park, N.; Yoon, M.; Berber, S.; Ihm, J.; Osawa, E.; Tománek, D. Magnetism in All-Carbon Nanostructures with Negative Gaussian Curvature. *Phys. Rev. Lett.* **2003**, *91* (23), 237204. <https://doi.org/10.1103/PhysRevLett.91.237204>.
- [4] Niu, W.; Ma, J.; Feng, X. Precise Structural Regulation and Band-Gap Engineering of Curved Graphene Nanoribbons. *Acc. Chem. Res.* **2022**, *55* (23), 3322–3333. <https://doi.org/10.1021/acs.accounts.2c00550>.
- [5] Chen, Z.; Narita, A.; Müllen, K. Graphene Nanoribbons: On-Surface Synthesis and Integration into Electronic Devices. *Adv. Mater.* **2020**, *32* (45), 2001893. <https://doi.org/10.1002/adma.202001893>.

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Poster 2

Modular Chemical Patterning of Graphene by Direct Laser Writing Using λ 3-Iodanes

Kevin Gerein¹, Diyan U. Dzujah², Hongde Yu², Frank Hauke¹, Tao Wei¹, Thomas Heine² and Andreas Hirsch¹

¹Center of Advanced Materials and Processes (ZMP) and Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

²Chair of Theoretical Chemistry, Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Dresden, Germany

The emerging laser writing represents an efficient and promising strategy for covalent 2D-patterning of graphene yet remains a challenging task due to the lack of applicable reagents. Here, we report a versatile approach for covalent laser patterning of graphene using a family of trivalent organic iodine compounds as effective reagents, allowing for the engraving of a library of functionalities onto the graphene surface. The relatively weak iodine-centered bonds within these compounds can readily undergo laser-induced cleavage to *in situ* generate radicals localized to the irradiated regions for graphene binding, thus completing the covalent 2D-structuring of this 2D film. Further insights into the reaction mechanism are gained by the assistance of theoretical calculations. The tailor-made attachment of distinct functional moieties with varying electrical properties as well as their thermally reversible binding manner enables precise programming of the surface properties of graphene. With this delicate strategy the bottleneck of a limited scope of functional groups patterned onto the graphene surface upon laser writing is tackled.

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Poster 3

2,2'-Diacetyl biphenyl as a precursor for porous graphitic carbon for electric double-layer capacitors

Aleena Jose, Julia Grothe and Stefan Kaskel

Department of Inorganic Chemistry, Technische Universität Dresden.

Porous graphitic carbon (PGC) frameworks are ideal electrode materials for electric double-layer capacitors (EDLC) because of their high surface area and conductivity. Reactive precursors with preset backbones can undergo graphitization at relatively lower temperatures to form conducting carbon with graphitic frameworks. Here, the triple aldol condensation of 2,2'-diacetyl biphenyl (2,2'-DAB) yielded a precursor which, when pyrolyzed at 800 °C, produced a microporous graphitic carbon framework (Figure 1) [1]. The small pore size of the PGC was found to be limiting the ion adsorption. Hence, we modified the framework by adding compounds with diacetyl groups like 1,4-diacetylbenzol (1,4-DABz) and 4,4'-diacetyl biphenyl (4,4'-DAB) along with 2,2'-DAB for increasing porosity. These modified PGC samples were measured for their capacitance as thin film electrodes in Swagelok cell assembly and were also used for the fabrication of simple in-plane micro supercapacitor structures using extrusion printing.

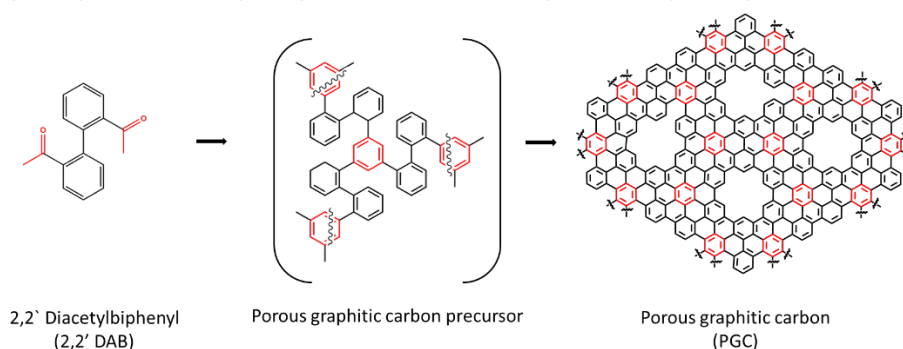


Figure 1. Scheme showing triple aldol condensation of 2,2'-DAB yielding the precursor which on pyrolysis yields the PGC.

References

[1] S. Che, C. Li, C. Wang, W. Zaheer, X. Ji, B. Phillips, G. Gurbandurdyev, J. Glynn, Z. Guo, M. Al-Hashimi, H. Zhou, S. Banerjee, L. Fang, *Chem. Sci.*, **2021**, 12, 8438.

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Visible-light responsive photo-switching HTI (Hemithioindigo) SAMs on surface

Jiwon Byun, Marcus Halik

Organic Materials & Devices, WW5, Friedrich -Alexander University

HTI (Hemithioindigo) chromophore and its derivatives exhibit visible light-responsive reversible photoisomerization between the E-isomer (favored at 420 nm) and Z-isomer (favored at 505 nm) configurations [1]. By functionalizing surfaces with these molecules, controlled molecular functions can be achieved, including unique photochromic properties. Attaching phosphonic acid groups to HTI chromophores enables the formation of HTI-SAMs (self-assembled monolayers), which can securely anchor to Al₂O₃ surfaces, ensuring stable adsorption and preventing issues such as island formation [2, 3]. To overcome the structural limitations of photo-switching behavior in the pure HTI SAM system, the integration of secondary supporting PAC6 (C6 alkyl chain with phosphonic acid) SAMs, forming HIT/PAC6 mixed binary SAMs system has optimized the photo-switching performance in the binary SAMs system on surface. This setup allows light-induced configuration changes in HTI-SAMs molecules to alter dipole moments at each isomeric state, thereby affecting surface potentials (Figure 1, left). Furthermore, integrating photo-switchable SAMs into field-effect transistors as a dielectric layer is anticipated to enable control of the capacitance corresponding to dipole moment changes [4, 5]. This leads to novel functionalities, such as reversible modulation of device performance using visible light.

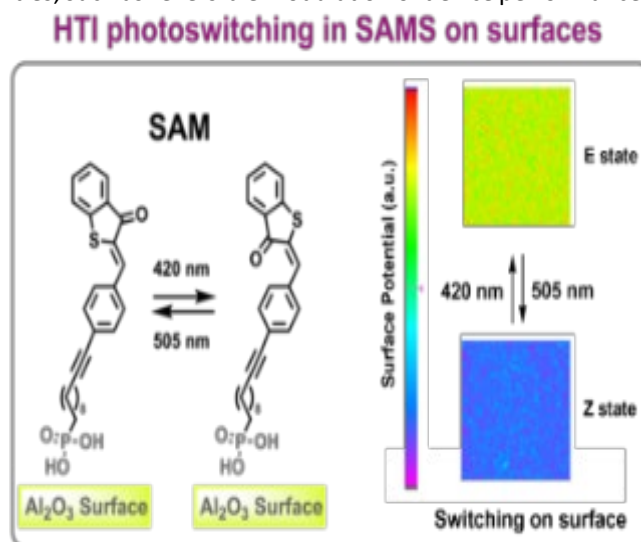


Figure 1: (left) HTI-SAMs molecules anchored on Al₂O₃ substrate; (right) surface potentials of each isomer's saturated states were measured by KPFM (box dimensions are 2.5 x 2.5 μm).

References

- [1] S. Wiedbrauk, and H. Dube. et al, *Tetrahedron Letters* 56.29 (2015): 4266-4274 (<https://doi.org/10.1016/j.tetlet.2015.05.022>)
- [2] T. Bauer, et al., *ACS Appl. Mater. Interfaces* 5.13 (2013): 6073–6080 (<https://doi.org/10.1021/am4008374>)
- b) H. Dietrich, et al., *Physical Chemistry Chemical Physics* 19.7 (2017): 5137-5144 (<https://doi.org/10.1039/C6CP08681K>)
- [3] Q. Shen, Qian, et al., *Advanced Materials* 22.30 (2010): 3282-3287 (<https://doi.org/10.1002/adma.201000471>)
- b) Y. Wang, Ye, et al., *ACS nano* 15.8 (2021): 13732-13741 (<https://doi.org/10.1021/acsnano.1c05167>)
- [4] A. Khassanov, et al., *Accounts of chemical research* 48.7 (2015): 1901-1908 (<https://doi.org/10.1021/acs.accounts.5b00022>)
- b) T. Schmaltz, et al., *ACS nano* 11.9 (2017): 8747-8757 (<https://doi.org/10.1021/acsnano.7b02394>)
- [5] A. Khassanov, et al., *Accounts of chemical research* 48.7 (2015): 1901-1908 (<https://doi.org/10.1021/acs.accounts.5b00022>)

Poster 6

Investigation of light-matter interaction under the environmental control of 2D materials via squeezable nanojunction technique

Sijia Feng, Heiko Weber

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Monolayers of transition metal dichalcogenides (TMDs), such as MoS₂, exhibit distinctive optical, electronic, and mechanical properties compared to their bulk or bilayer counterparts. In particular, monolayer TMDs possess a larger direct bandgap, leading to higher energy absorption and stronger photoluminescence (PL) emission. In this study, we utilize the squeezable nanojunction (SNJ) technique to systematically investigate the evolution of PL properties as two MoS₂ monolayers are gradually brought into contact to form a bilayer. By precisely controlling the nanoscale separation between the monolayers, we continuously monitor the PL signal at each stage, providing key insights into the transition from monolayers to a bilayer structure.

Specifically, we measure the PL response from both individual monolayers and the overlapping region as the interlayer distance decreases incrementally. This approach allows us to capture the complete evolution of PL changes as the system transitions from two separated monolayers to a bilayer, where interlayer coupling and excitonic effects become significant. Our findings reveal detailed shifts in PL intensity and spectral features, elucidating the optical transition from monolayer TMDs to the bilayer structure.

This research offers a comprehensive framework for exploring interlayer coupling, exciton dynamics, and potential modifications in band structure within 2D TMD heterostructures. Future studies may extend this method to other TMD systems or examine the effects of parameters such as material composition, twist angle, and substrate influence on PL behavior during the formation of both heterostructures or bilayers.

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Poster 7

Prediction of core-level satellites from highly accurate Green's function methods

Jannis Kockläuner, Dorothea Golze

Chair of Theoretical Chemistry, Dresden University of Technology

Satellites arise due to collective charged and charge neutral excitations which can gain significant spectral weight in extended systems. Since satellites arise due to many-body processes, the theoretical prediction requires correlated approaches like the *GW* method. However, the neglect of vertex corrections in *GW* creates spurious satellite features in the spectral function.[1] In this work, we employ the *GW+C* method for the accurate prediction of satellites and extend it to core-level spectra of molecules. We have implemented this approach as a post-processing tool in the FHI-aims code, enabling large-scale calculations with more than 3,000 orbitals. We find excellent agreement with experimental data for large molecules such as porphyrins.

[1] Zhou, J. S., et al., J. Chem. Phys., 143(18), (2015).

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Poster 8

Interfacial charge transfer states: a study in dispersion and solid state

Elena A. Mack¹, Alejandro Cadranel¹, Kevin Synnatschke², Leandro Lourenço³, Dirk M. Guldi¹

¹Friedrich-Alexander-Universität (Germany), ²Technische Universität Dresden (Germany), ³University of Aveiro (Portugal)

Solution-processed nanosheet networks (NN) of exfoliated transition metal dichalcogenides (TMDs) have attracted immense interest which is partially attributed to their compatibility with printing techniques, suitable for large area processing. The electrical characteristics of the NN obtained from liquid–liquid interface deposition, demonstrate an electron mobility of $10 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ for networks of molybdenum disulfide nanosheets [1]. The TMD NN's semiconducting nature offers opportunities for adjusting electronic properties through functionalization, especially with thiopyridyl-cobalt phthalocyanines (CoPcs). These molecular building blocks have previously demonstrated effectiveness in carbon capture mechanisms [2].

Here, we report on non-covalent functionalized TMD NN with CoPcs immobilized on the exposed basal plane surface of the NNs [3]. The appearance of charge transfer (CT) steady-state extinction bands imply strong ground state interactions between TMDs and CoPc. The interfacial CT states have electronic matrix coupling elements of about 1000 cm^{-1} , which is rather typical for strongly coupled CT systems. Electrochemical characterizations show distinct peaks for the functionalized films, confirming that the CoPcs act as electrochemically active sites on the surface of the NN. Furthermore, charge separation was corroborated by femtosecond transient absorption spectroscopy [4] supported by steady-state spectroelectrochemistry of the CoPcs. We hence conclude that these NNs exhibit favorable characteristics for tailored design of catalytic systems.

References

[1] Kelly, A. G., O'Suilleabhain, D., Gabbett, C., & Coleman, J. N., *Nature Reviews Materials*, 7, 217–234 (2022). [2] Roy, S., Miller, M., Warnan, J., Leung, J. J., Sahm, C. D., & Reisner, E, *ACS Catalysis*, 11, 1868–1876, (2021). [3] Wibmer, L., Lourenço, L. M. O., Roth, A., Katsukis, G., Neves, M. G. P. M. S., Cavaleiro, J. A. S., Tomé, J. P. C., Torres, T., & Guldi, D. M., *Nanoscale*, 7, 5674–5682 (2015). [4] Scharl, T., Binder, G., Chen, X., Yokosawa, T., Cadranel, A., Knirsch, K. C., Spiecker, E., Hirsch, A., & Guldi, D. M., *Journal of the American Chemical Society*, 144, 5834–5840 (2022).

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Poster 9

2D conjugated metal-organic framework for quantum information science.

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Quantum computing has the potential to reshape the future industries by promising faster solutions for optimization, simulation and machine learning problems [1]. As basic unit of quantum computing, qubits are the quantum version of the classical binary bit [2]. Among all their physical realization, molecular electron spin qubits based on π -conjugated molecules offer interesting properties such as a long spin lifetime and diffusion length [3-5]. However this type of system suffers from a poor air stability and lacks of an effective molecular arrangement [6]. To address those challenges, our work is focused on the synthesis of 2D conjugated metal organic frameworks showing stable unpaired electron assembled in a periodic structure. Through the specific design of the conjugated ligands and the selection of the appropriate metal ion, the spin properties of the material are tuned and allows the exploration structure-properties relationship.

[1] *Nature* 574, 505-510 (2019); [2] *Nature Reviews Chemistry* 4, 490-504 (2020); [3] *Nature Materials* 8, 693–695 (2009) [4] *Nature Chemistry* 11, 301–309 (2019); [5] *Journal of the American Chemical Society* 2024 146 (4), 2574-2582 [6] *ACS Nanoscience Au* 2022 2 (4), 333-340

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Spatially resolved 2D Laser Writing of Graphene with Diazonium Salts

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Modifying graphene *via* covalent functionalization by introducing various functional moieties and therefore tuning the chemical properties has established itself as a key field in graphene research.^[1] Modern 2D patterning techniques, which combine highly efficient, covalent functionalization with precise spatial resolution, allows a dimensional and quantitative control over the addend binding.^[2] Herein, we present an optimized protocol for the laser-activated spatially resolved functionalization of graphene using various diazonium salts exhibiting different functional groups, where the laser writing behavior of 4-*tert*-butylbenzenediazonium tetrafluoroborate (4-TBBD) is presented in detail.

References

[1] T. Wei, F. Hauke, A. Hirsch, *Adv. Mater.* **2021**, *33*, 2104060.

[2] K. F. Edelthammer, D. Dasler, L. Jurkiewicz, T. Nagel, S. Al-Fogra, F. Hauke, A. Hirsch, *Angew. Chem. Int. Ed.* **2020**, *59*, 23329-23334.

Poster 11

Towards Highly Controlled 2D-Engineering of Graphene

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Covalent functionalization of graphene is a powerful tool to tune the materials unique properties. The development of various methods to achieve locally controlled modifications was a tremendous step towards tailor-made graphene based materials. Herein, we present a fundamental study regarding the laser-activated spatially resolved functionalization of graphene using dibenzoyl peroxide (DBPO) as model compound with an unprecedented level of control. By adjusting the parameters, we have precise control over the degree of functionalization, are able to generate structures down to 1 μm in size and by combining our technique with a mask-assisted approach, the resolution can even be improved beyond 300 nm. To demonstrate the reversibility of the covalent functionalization, we present two pathways to induce defunctionalization using either heat or high power laser irradiation as the stimulus. As the next step, we established an iterative laser writing procedure allowing for secondary functionalization side by side or across prior functionalized areas, as well as on beforehand locally defunctionalized areas.

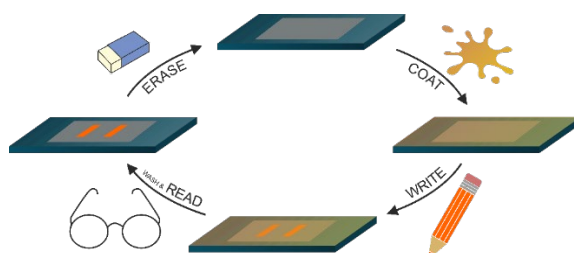


Figure 1. Schematic representation of the coat - write - read - erase cycle.

References

- [1] C. Wetzl, et al, *Angew. Chem. Int. Ed.* **2023**, 62, e202212857
[2] K. F. Edelthammer et al, *Angew. Chem. Int. Ed.* **2020**, 59, 23329-23334.
[3] H. Liu et al, *J. Am. Chem. Soc.* **2009**, 131, 1709917101.
[4] T. Nagel et al, *manuscript in preparation*.

Poster 12

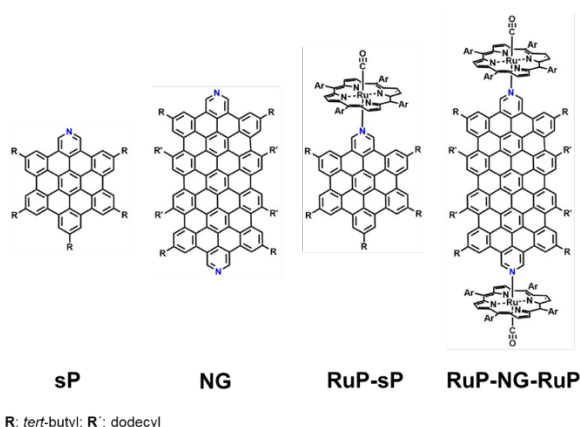
Lateral π -extended molecular nanographene

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Molecular nanographenes represent a promising candidate for optoelectronics and energy applications, in view of their intriguing and tunable properties [1]. We report [2] on the rich photophysics and self-assembly behaviour of two nitrogen-containing fully benzenoid nanographenes: azananographene **sP**, which features a hexa-peri-hexabenzocoronene (**HBC**) core, and diazananographene **NG**, which can be regarded as a laterally π -extended **sP**. The lateral π -extension of the aromatic core when going from **sP** to **NG**, resulted in an intriguing modulation of the photophysical properties, alongside with the rise of self-assembly behaviour. For example, **NG** shows a fluorescence quantum yield of 60% and thermally activated dual fluorescence from both S_1 and S_2 . Our work was rounded off by coordinating ruthenium porphyrins (**RuP**) to the nitrogen centers of **sP** and **NG**, leading to **sP-RuP** and **RuP-NG-RuP**. In **sP-RuP** an ultrafast energy transfer from the singlet excited state of **sP** to **RuP** is observed. Instead, in **RuP-NG-RuP** a "ping-pong" energy transfer, namely from **NG** to **RuP** and back to **NG**, is reported. Lastly, **NG** self-assembles in solution into dimers and then into highly ordered 2D supramolecular structures, with great potential for optoelectronic applications.

References

- [1] Z. Liu *et al.*, *Adv. Sci.* 9, 2106055 (2022).
[2] G.M. Beneventi *et. al.* *Adv. En. Mat.* 14, 2401529 (2024).

Poster 13

On-surface synthesis and study of GNRs with defect lines

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Graphene nanoribbons (GNRs) have drawn significant attention in recent decades due to their extraordinary electronic properties such as tunable band gap [1], making them promising candidates for integration into nanoelectronics [2]. Density functional theory (DFT) calculations suggest that the introduction of defect lines, such as 4-8 membered rings into GNRs, gives rise to distinct families of semiconducting or Dirac-like behavior [3], making these ribbons both physically and electronically appealing. Bottom-up on-surface synthesis under ultrahigh vacuum conditions is a promising approach for fabricating these kinds of ribbons. In our research, we aim to synthesize GNRs with varying defect lines using paracyclophanes derivative as the precursor and to investigate their characteristic structural and electronic properties using scanning tunneling microscopy and spectroscopy.

References

- [1] O. Roslyak, G. Gumbs, and D. Huang, "Tunable band structure effects on ballistic transport in graphene nanoribbons," *Physics Letters A* 374(39), 4061–4064 (2010).
- [2] B. Obradovic, R. Kotlyar, F. Heinz, P. Matagne, T. Rakshit, M.D. Giles, M.A. Stettler, and D.E. Nikonov, "Analysis of graphene nanoribbons as a channel material for field-effect transistors," *Applied Physics Letters* 88(14), (2006).
- [3] R. Gillen, and J. Maultzsch, "Family behavior and Dirac bands in armchair nanoribbons with 4–8 defect lines," *J. Phys.: Condens. Matter* 36(29), 295501 (2024).
- [4] M. Liu, M. Liu, L. She, Z. Zha, J. Pan, S. Li, T. Li, Y. He, Z. Cai, J. Wang, Y. Zheng, X. Qiu, and D. Zhong, "Graphene-like nanoribbons periodically embedded with four- and eight-membered rings," *Nat Commun* 8(1), (2017).

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Poster 14

Processing Chitin-Graphene Oxide into Stable Composite Materials for Efficient Heavy Metal Adsorption from Aqueous Solution

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Rare earth elements (REEs) are vital to modern technology due to their unique properties and widespread industrial use. However, their increased use raises environmental and health concerns due to bioaccumulation and toxicity. Efficient removal of REEs from aqueous waste streams, mainly from radioactive waste in the aquatic nuclear industry, is critical. Recycling these elements has emerged as a sustainable approach to waste reuse and wastewater processing. Various reported methods were developed for removing heavy metal ions from wastewater sources. Currently, adsorption is a standard method for water purification and wastewater treatment. Adsorption depends on the physical and chemical interactions between heavy metal ions and adsorbents. Primary properties of suitable adsorption methods are (i) high adsorption efficiency and capability of removing different ion types, (ii) high retention time and cycling stability of adsorbents, and (iii) availability. Large amounts of crab and prawn shells are abandoned, and the possibility of developing value-added products from these remnants is of interest. Chitin is a commercially available biopolymer from marine waste. Chitin exhibits several favorable properties: availability, low cost, high biocompatibility, and biodegradability. These properties make it biologically and chemically interesting for various applications. It is also well known that chitin effectively adsorbs metal ions, including uranium and other toxic heavy metals. However, processing chitin into stable structures, e.g., composite chitin-based composites, is challenging due to its high chemical stability and extremely low

solubility. In our previous research, α -chitin processed with IL 1-Butyl-3-methylimidazoliumacetate showed a lower adsorption capacity due to the partial blocking of adsorption sites. To overcome this, we incorporated graphene oxide (GO) into the chitin matrix. With its large surface area and functional groups, GO brings a unique and innovative approach to improved composite adsorbents. In this study, we processed α -chitin extracted from shellfish and graphene oxide in 1-Butyl-3-methylimidazoliumacetate to create chitin-GO-based composites. These composites, with their potential to serve as heavy metal ion adsorbents, were the focus of our investigation. We characterized the materials before and after Eu (III) adsorption using scanning electron microscopy, Fourier-transform infrared spectroscopy, and NMR spectroscopy. Eu (III) was chosen as a non-radioactive representative and analog for other f-elements, and its adsorption was quantified using ICP-OES. Favorable adsorption capacities are observed.

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Poster 15

Local Electric Fields at Planar Carbon-based Electrodes

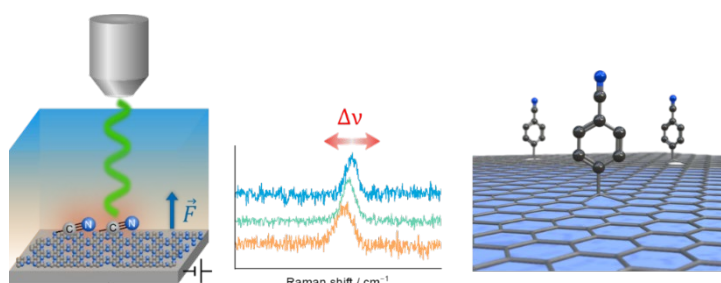
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Short-ranged electric fields at electrode surfaces play an important role within an electrocatalytic cycle. These fields can be measured via the Vibrational Stark Effect (VSE), which arises from the interaction between a local electric field \vec{F} and a vibrational mode of a surface-bound molecular group, resulting in characteristic frequency shifts $\Delta\nu$. Project C5 of RTG-2861 aims to investigate local electric fields at 2D carbon electrodes containing VSE-reporter groups using *in-situ* spectroelectrochemical methods.

First, a C_2N -type carbon material active for electrocatalytical hydrogen evolution reaction (HER) is investigated under non-turnover conditions and inherently bound nitrile groups are found to act as Stark reporter groups, displaying a linear frequency shift with applied electric potential. During HER, a deviation from the linear Stark shift is observed that implies a conditioning of the electrode due to the catalytic turnover.

Second, graphene is covalently functionalised with nitrile-containing groups and the characteristic $\text{C}\equiv\text{N}$ stretching mode is observed in the Raman spectra. Possible frequency shifts under applied electric potential according to the VSE are currently under investigation and could provide insights into the electric field environment at the heterogeneous interface of metal-free carbon electrodes.

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