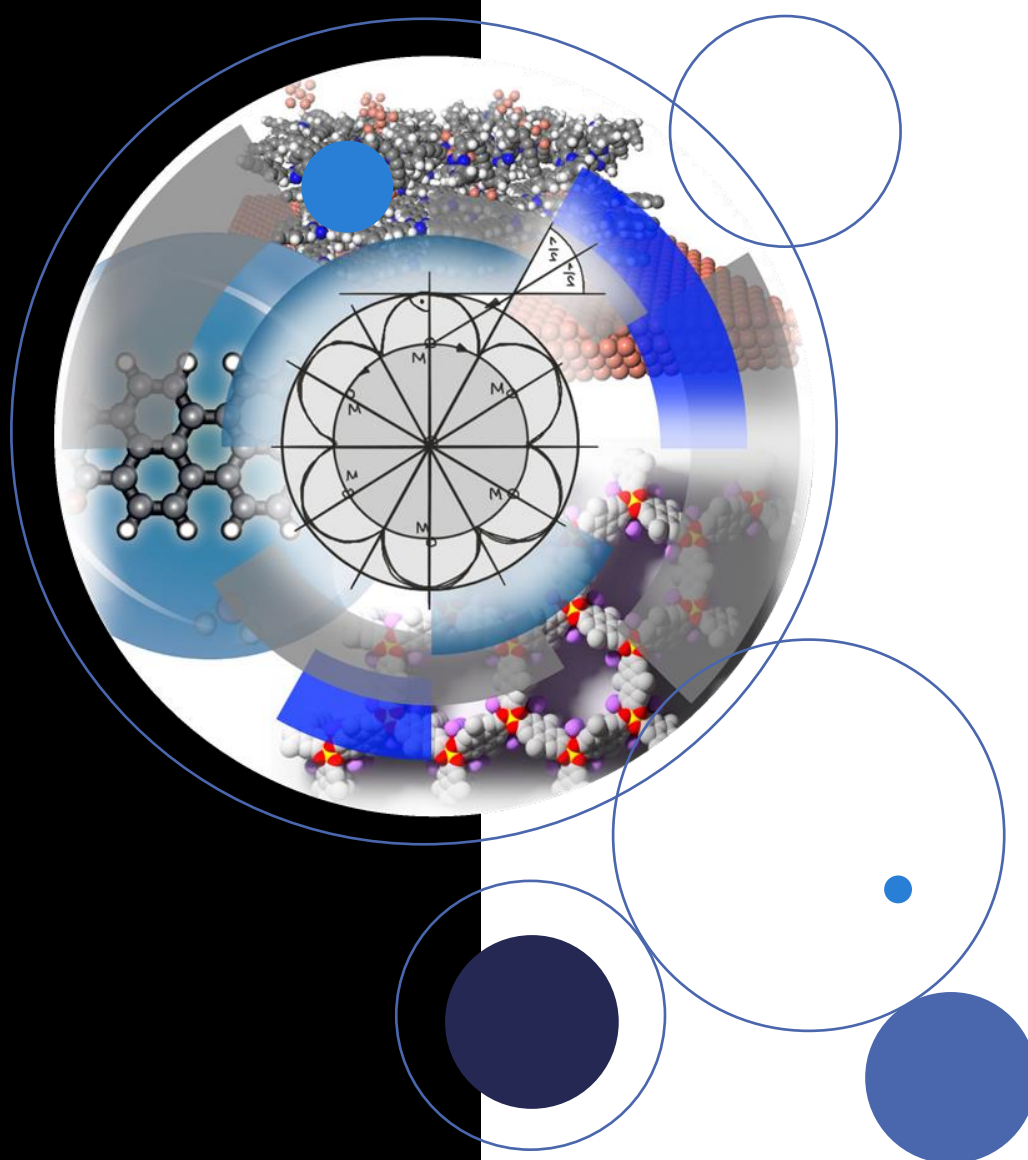


Functional Nanomaterials Symposium



#FuNMat2019
17-19 May, Berlin



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WILEY-VCH

NEWS: "Publish and Read" contract with Wiley concluded

January 15, 2019

Germany's Projekt DEAL and the publisher John Wiley & Sons have entered a ground-breaking transformative agreement, in line with the objectives of the Open Access 2020 initiative.

Projekt DEAL, a representative of nearly 700 academic institutions in Germany, and Wiley announced today a countrywide partnership agreement. Under an annual fee, this transformative three-year agreement provides all Projekt DEAL institutions with access to read Wiley's academic journals back to the year 1997, and researchers at Projekt DEAL institutions can publish articles open access in Wiley's journals.

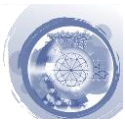




PROGRAM

REGISTRATION – 17.05. (Fri) from 8 am

	17.05. (Fri)		18.05. (Sat)	19.05. (Sun)
09:00	p3 A. Clemens*		p19 M. Unterlass* (TU Vienna)	p37 T. Hasell* (U Liverpool)
15+5			Generating fully heterocyclic and aromatic materials hydrothermally	Catalytic inverse vulcanisation
09:20	[WORKSHOP] How to use story-telling in a scientific paper	Founding ceremony of the FuNMat e.V. (founding members only)	p20 D. A. Cerrón-Inf. (TU Vienna)	p38 A. P. Periasamy (QMUL)
15+5			Polyimide processing from aqueous solutions	Synthesis of nitrogen doped porous carbon microspheres using metal assisted polymerization strategy for efficient oxygen reduction reaction
09:40			p21 A. Acharjya (TU Berlin)	p39 M.-Y. Ye (TU Berlin)
15+5			Olefin-linked covalent organic frameworks (COFs)	Cobalt-exchanged poly(heptazine imides) as transition metal-Nx electrocatalysts for oxygen evolution reaction
10:00	p4 M. J. Bojdys (HU Berlin)		p22 T.-P. Fellingner (TU Munich)	p40 K. Skrodzky (HU Berlin)
15+5	Welcome and Introduction - Leadership 4.0: Succeeding in a new era of transparency and data-flow		Active-site imprinting towards tailored carbon electrocatalysts	Nanosized niobium pentoxide acid catalysts with varying acidity: Insights into the structure-acidity-activity relationships of Nb ₂ O ₅
10:20	p5 J. Roeser (TU Berlin)		p23 L. Tran (QMUL)	p41 M. Qiao (Imperial)
15+5	3D anionic silicate covalent organic framework with srs topology		Composite of spinel NiFe ₂ O ₄ and heteroatom doped carbon fibre derived from lignin as bifunctional oxygen electrocatalyst	Water-equilibrated high-O ₂ -soluble ionic liquids make nanocarbon more active and stable for oxygen reduction catalysis
10:40	p6 H. Moura (TU Vienna)		p24 R. L. Upton (U Liverpool)	p42 J. A. Smith (U Liverpool)
15+5	Perylene bisimide@zeolite hybrid materials by one-pot hydrothermal synthesis		Superhydrophobic materials fabrication using polymer-nanoparticle composites	Inverse vulcanised sulfur polymers for functional materials
11:00	p7 A. Martin (HU Berlin)		p25 X. Han (HU Berlin)	p43 F. Xie (Imperial)
15+5	Iron fluoride phases towards alkali ions des/insertion		Nonaqueous synthesis of Nb ₂ O ₅ @carbon nanoparticles and nanospheres for high performance hybrid supercapacitors	Hard-soft carbon composite anodes with synergistic sodium storage performance
11:20	p8 A. Valencia (HU Berlin)		p26 Z. Xu (Imperial)	p44 I. Ilic (MPI KGF)
15+5	Electronic and optical properties of oligothiophene-F4TCNQ charge-transfer complexes: the role of donor conjugation length		All-cellulose-based quasi-solid-state sodium-ion hybrid capacitors enabled by structural hierarchy	Vanillin-based polymer as a sustainable alternative for cathodes in lithium-ion batteries
11:40	p9 J. Allen* (Chemical Science)		p27 R. Kulkarni (HU Berlin)	p45 M. J. Bojdys (HU Berlin)
15+5	My role within a societal publisher and tips on how to publish your scientific research		A real-time optical and electronic chemical sensor based on triazine-containing 2D materials	Closing remarks and best student-talk award (by Wiley-VCH)
12:00	Lunch		Lunch	
14:00	p10 A. Thomas* (TU Berlin)		p28 M. Titirici* (Imperial)	
15+5	Functional nanoporous materials for unifying systems in catalysis		Sustainable is the new black	
14:20	p11 T. Cavalli (TU Vienna)		p29 S. Bhatia (FU Berlin)	
15+5	Controlling the crystallization of all-organic salts		Polyglycerol based broadly active multivalent inhibitors of influenza virus	
14:40	p12 D. Burmeister (HU Berlin)		p30 M. M. Iqbal (TU Vienna)	
15+5	Birth of a 2D material		Synthesis of high-performance covalent organic frameworks via a green hydrothermal route	
15:00	p13 M. Guerrini (HU Berlin)		p31 A. Vogel (U Liverpool)	
15+5	Intra- and intermolecular charge transfer in the optical excitations of J-aggregates formed by push-pull chromophores		Ladder polymers for hydrogen evolution from water	
15:20	p14 J. Huang (HU Berlin)		p32 S. Vogl (TU Berlin)	
15+5	Fully aromatic, covalent phosphinine frameworks: from synthesis to application		Tailor-made carbazole-based microporous polymer networks for photocatalytic applications	
15:40	p15 M. Citroni* (Nat. Commun.)		p33 M. Crespo (QMUL)	
15+5	Producing impactful science: general guidelines for day to day research		Lignin-derived electrospun freestanding carbons as alternative electrodes for RFB	
16:00	Coffee		Coffee	
17:00	p16 C. Cocchi (HU Berlin)		p34 E. List-Kratochvil* (HU Berlin)	
15+5	An illuminating perspective on nanomaterials from ab initio electronic structure theory		Printed functional nanomaterials for optoelectronic applications	
17:20	p17 S. Hérou (Imperial)		p35 F. A. Amaya-García (TU Vienna)	
15+5	Low-cost carbon nanofiber textiles as free-standing electrodes in supercapacitors		Implementing hydrothermal synthesis for novel fluorescent cell-staining dyes	
17:40	p18 Y. Lu* (HZB)		p36 H. Bildirir (Chalmers)	
15+5	Block copolymer template-directed synthesis of well-ordered composite nanostructures		Triplet-triplet annihilation photon upconversion via macromolecular annihilators	
18:00	Dinner		Dinner	



How to use story-telling in a scientific paper

Anna Clemens »Scientists Who Write«, Prague, Czech Republic

Human brains love stories – we have evolved to pay attention to them. We get more emotionally involved with a story and remember it better than a list of facts. However, many scientists don't make use of the power of story-telling when they are reporting their findings in a paper. In this talk, I'm going to show you which story elements used in dramas are also essential in a scientific paper, and how to use them when writing an abstract. You will learn to master a 6-step process, which will allow you to consistently write perfect abstracts for papers and conferences. Understanding how you can use story-telling to structure your abstract and paper will help you to communicate your scientific findings in a simple and clear way – the key to getting your excellent research funded and published in high-impact papers.

Anna Clemens holds a PhD in Materials Science and is a scientific writing coach, editor and freelance science writer. She helps her clients to write high-impact papers and win grant proposals. She has been published in various popular science magazines, e.g. *Scientific American* and *Spektrum der Wissenschaft*.

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Instagram: [@scientistswhowrite](https://www.instagram.com/scientistswhowrite)

IMPORTANT NOTE: participants should bring their laptop and any recent abstract (electronic version, for a paper or conference) to Anna's session.



Leadership 4.0: Succeeding in a new era of transparency and data-flow

Michael J. Bojdys, Department of Chemistry, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany

In many respects we are still conducting experimental research in our labs like 150 years ago. Researchers weigh in and transfer colourful powders and liquids by hand, we sway and shake round bottles and conical flasks, and people doodle in their lab notes using pen and paper in a more-or-less legible fashion. It looks like manufacturing. And just like manufacturing was superseded by more productive, industrial processes at the end of the 19th century we see the same trends of automation and digitalisation taking hold in laboratories and in industrial chemistry.

One might rightly question whether the scientific process needs automation at all. Was it not genius individuals, remarkable women and men, who made the biggest discoveries of human kind; people who we as the scientific community dignify with the highest honours? The “industrial revolution of science” is not putting these remarkable individuals at risk – genius ideas will still be needed in the future. But science does not exist in a social vacuum, and we researchers have a unique responsibility in times of “fake news” and scepticism to bring ourselves and our findings into society.



Supported by European Research Council (ERC) under the Starting Grant scheme (BEGMAT – 678462).



3D anionic silicate covalent organic framework with srs topology

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Arne Thomas^a

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Covalent organic frameworks (COFs) have emerged as an important class of materials and hold the promise for improved performance in applications such as gas storage and separation, heterogeneous catalysis, proton and ion conduction or optoelectronics.¹ As with any class of materials, COFs would benefit from increased compositional and structural complexity and a major challenge in the development of this class of material lies in the expansion of linkages (bonds formed to reticulate the building blocks), composition and topologies (underlying nets describing such frameworks). In terms of structure, the field is dominated by 2D COFs and most of the COFs reported consist of extended 2D layers stacking up in the third direction to form an overall 3D framework with unidirectional pore channels. 3D COFs have been developed to a lesser extent, especially in terms of accessible topologies and so far 3D COFs were only reported for nets based on building blocks with tetrahedral geometry.

Here, we report the synthesis of SiCOF-5, a 3D anionic COF crystallizing in the three-coordinated (3-c), two-fold interpenetrated, **srs-c** net, one of the five regular nets described in the reticular chemistry structure resource (RCSR) but never reported for COFs. Our strategy consists in exploiting a new linkage recently developed in our laboratory by implementing reversible Si-O chemistry for the reticulation of ditopic catecholate linkers around dianionic hexacoordinate silicon vertices.² A key requirement for the crystallization of SiCOF-5 was the careful control over the nucleation and growth rate by gradual generation of silicon source during the course of the reaction.³

¹ C. S. Diercks et. al, *Science* **2017**, 355, eaal1585. DOI: 10.1126/science.aal1585

² J. Roeser et. al, *Nat. Chem.* **2017**, 9, 977. DOI: 10.1038/nchem.2771

³ O. Yahiaoui et. al, *J. Am. Chem. Soc.* **2018**, 140, 5330. DOI: 10.1021/jacs.8b01774



Perylene bisimide@zeolite hybrid materials by one-pot hydrothermal synthesis

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^b*Institute of Applied Synthetic Chemistry, TU Wien, Getreidemarkt 9, 1060, Vienna, Austria,*

^c*CeMM- Research Center for Molecular Medicine of the Austrian Academy of Sciences, Lazarettgasse 14, 1090 Vienna, Austria*

Hybrid materials (HMs) consisting of organic photoactive dyes embedded in an inorganic host are promising materials for light-harvesting and solar energy transport applications.¹ Here, zeolites are most promising host materials, because their pores can (i) act as ideal spaces for incorporating organic dyes, and (ii) the small pore sizes potentially counteract dye aggregation. Organic perylene bisimide (PBI) dyes are interesting as guests, since they show high photostability and fluorescence quantum yields.² However, synthetic routes towards PBIs@zeolites are to date exclusively based on multistep reactions. These classical routes usually result in poor control over the organic-inorganic interface, as well as leaching out from and/or poor dispersibility of the dye within the pores of the host zeolite. In this contribution, we present a one-pot approach aimed at circumventing these drawbacks by simultaneous synthesis of the two components. We show that PBI@zeolite HMs can be generated simultaneously by hydrothermal synthesis (HTS). HTS is a classical method used to generate inorganic materials such as zeolites and gemstones. Recently,^{3,4} we showed that organic dyes can also be prepared by HTS. Here, we use HTS to prepare PBI@zeolite HMs, and discuss the products' materials properties arising from the simultaneous synthesis.

Supported by the Austrian Science Fund (FWF) under the Grant "HYDROCOF – The hydrothermal route to covalent organic frameworks" (START Y1037-N28)

¹ S. H. Mir et. al. *J. Electrochem. Soc.* **2018**, 165, 3137. DOI: 10.1149/2.0191808jes

² P. Cao et. al. *Chem. Eur. J.* **2016**, 22, 4046. DOI: 10.1002/chem.201504404

³ B. Baumgartner et. al. *Chem. Commun.* **2017**, 53, 1229. DOI: 10.1039/C6CC06567H

⁴ M. J. Taublaender et. al. *Angew. Chem. Int. Ed.* **2018**, 58, 12270. DOI: 10.1002/anie.201801277



Iron fluoride phases towards alkali ions des/insertion

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Li-ion batteries (LIBs) are omnipresent in consumer electronics and are seen as the most promising technology for electrical vehicles. Na-ion batteries (NIBs) have emerged as viable and cheaper alternatives for stationary applications where Li-ion batteries are too expensive. However, the larger size of sodium ion compared to lithium makes traditional positive materials for LIBs not always suitable for the reversible insertion of sodium ions. 3d-transition metal fluorides, such as FeF_3 , have drawn attention as NIBs and LIBs positive electrode material due to their ability to deliver high potential thanks to the high polarity of the metal-fluorine bond. However, the insulating character of these highly ionic materials in practice leads to high polarisation and slow insertion kinetics.¹⁻³ The anhydrous hexagonal FeF_3 shows acceptable performances, but the latter are hindered by complicated insertion/conversion reactions when this crystalline phase reacts toward 1Li. Another side, the pathway of reaction followed by the metal fluoride perovskites (NaFeF_3 and KFeF_3) kinetically favored, allows the straight insertion of alkali ions within the structure, enabling low polarisations and exceptional rate capabilities. The charge/discharge processes are herein studied through ex-situ and operando X-ray diffraction measurements, for the hexagonal and perovskite nanosized compounds, to understand the mechanisms related to the respective electrochemical behaviors. This mechanistic study is as well supported by polymorphism theoretical analysis.⁴

¹ D. E. Conte, N. Pinna, *Mater. Renew. Sustain. Energy*, **2014**, 3, 37

² L. Di Carlo, D. E. Conte, E. Kemnitz, N. Pinna, *Chem. Commun.*, **2014**, 50, 460

³ D. E. Conte, L. Di Carlo, M. T. Sougrati, B. Fraisse, L. Stievano, N. Pinna *J. Phys. Chem. C*, **2016**, 120, 23933

⁴ A. Martin, M.-L. Doublet, E. Kemnitz, N. Pinna, *Adv. Funct. Mater.*, **2018**, 1802057.



Electronic and optical properties of oligothiophene-F4TCNQ charge-transfer complexes: the role of donor conjugation length

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^aPhysics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Zum Großen Windkanal 6, 12489 Berlin, Germany

We investigate a series of charge transfer complexes formed by oligothiophene (nT) molecules doped by the acceptor F4TCNQ, in order to understand the role of donor conjugation length. Using hybrid DFT as a starting point, we compute the electronic and optical properties of these systems from many-body perturbation theory (GW approximation and the Bethe-Salpeter equation). We find that the frontier orbitals (HOMO and LUMO) are hybridized in all complexes, while the distribution of deeper occupied and higher virtual states depends on the nT length. The first bright excitation is dominated by the HOMO-LUMO transition occurring approximately at the same energy in all systems. At increasing donor length, higher-energy peaks exhibit different character depending on the donor conjugation length. The rationale offered by our results contributes to clarify the excitation processes in organic donor/acceptor complexes.¹

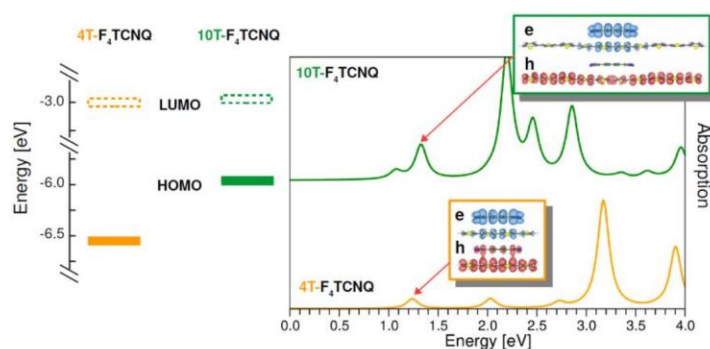


Figure 1. Level alignment, optical spectra, and electron (e) and hole (h) densities of oligothiophene-based charge-transfer complexes. Taken from Ref.¹

Supported by the Deutsche Forschungsgemeinschaft (DFG) - Projektnummer 182087777 - SFB 951 – and HE 5866/2-1.

¹ A.M. Valencia and C. Cocchi J. Phys. Chem. C 2019, in press DOI:10.1021/acs.jpcc.9b01390



My role within a societal publisher and tips on how to publish your scientific research

*Jeremy P. Allen, Chemical Science, Royal Society of Chemistry, Thomas Graham House,
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The Royal Society of Chemistry is one of the leading international chemical societies and it plays an important role within the community – helping to support those working in and studying the chemical sciences with a wide range of activities. During this presentation I will introduce the work that the Royal Society of Chemistry does, my role within the organization and the route I took from PhD student to being the Deputy Editor for Chemical Science. I will also highlight the role publisher's play in the community and the benefits they can afford for supporting the dissemination of an author's research output. Finally I will discuss the peer review and publication process, including how to choose a journal, getting your paper noticed and what to do after publication.



Functional nanoporous materials for unifying systems in catalysis

Amitava Acharjya,^a Nicolas Chaoui,^a Esteban G. Gioria,^a Julia Grüneberg,^a Daniel Hagemeyer,^a Michaela König,^a Sophie Kücken,^a Thomas Langenhahn,^a Changxia Li,^a Shuang Li,^a Rafael de Lima,^a Pradip Pachfule,^a Jerome Roeser,^a Johannes Schmidt,^a Sarah Vogl,^a Vincent Weigelt,^a Jin Yang,^a Meng-Yang Ye,^a Xiaojia Zhao,^a Arne Thomas^a

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Catalysis is a key technology of utmost importance for the economic and ecological welfare of societies because it is the decisive part of developing resource-saving and sustainable processes for energy and materials conversion. Porous functional materials having large accessible surface areas and defined functionalities on their surface play a key role as catalysts for a range of viable reactions. However, catalytic processes can be highly diverse and thus the nature and properties of suitable catalysts can strongly differ. As example, many important industrial reactions require harsh conditions, making inorganic materials such as zeolites or mesoporous oxides the matter of choice. On the other hand, electro- or photocatalytic conversions, urgently needed for a future sustainable economy, require abundant and conducting or semiconducting substrates, making carbon or carbon nitride-based catalysts interesting. Finally porous organic materials are ideal candidates to unify homogeneous and heterogeneous catalysis in a range of important catalytic reactions. In these materials molecular catalysts are immobilized by polymerizing them into open framework structures. The talk will give an overview on the materials and catalyst developments in the *Functional Materials* group and a short insight into the newly founded Cluster of Excellence *UniSysCat* in the Berlin area.

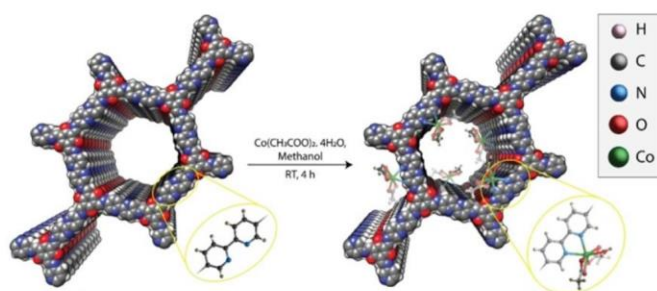


Figure 1. Immobilization of a Co-bipy catalyst in a Covalent Organic Framework with bipyridine linkers



Controlling the crystallization of all-organic salts

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Organic salts are virtually omnipresent in chemical products, spanning from pharmaceuticals to food additives and colorants. The manufacturing of organic salts typically involves several steps where they are handled in the form of solid, crystalline powders. The powder form, *i.e.* crystal structure, size and shape of the salt particles, is extremely important for the production processes, as it affects aspects such as powder drying or flowability. Therefore, exerting control over the powder form of organic salts is highly desired. While nucleation and crystallization of simple inorganic salts – such as the prototypical CaCO_3 – are well studied and relatively well understood,¹ crystallization of all-organic salts is heavily understudied, which is most likely due to the fact that all-organic salt nucleation involves a multitude of species in solution, making them a highly complex subject of study.

We herewith present our efforts to understand and control the crystallization of all-organic salts (*i.e.* salts where both anion and cation are organic molecules). These systems are hardly controllable, as all-organic salts are typically rich in non-covalent interactions (NCIs) in their crystalline forms, which often renders them sparsely soluble and imparts nucleation at high supersaturation. At the hand of a highly insoluble model salt, we show how control over size and shape can indeed be achieved by different crystal growth techniques, including the use of additives. Moreover, we discuss the physicochemical underpinnings for the generated control, both in solution (*i.e.* pre-nucleation), and in the solid state.

Supported by TU Wien in the framework of the doctoral school "BIOINTERFACE"

¹ F. C. Meldrum, H. Cölfen, *Chem. Rev.* **2008**, 108 (11), 4332–4432.



Birth of a 2D material

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Reaching the limits of silicon based semiconductor technology, the end of Moores law comes closer. Therefore materials for post silicon electronics are highly demanded to sustain the ongoing digital revolution. These materials potentially enable the further miniaturisation of electronic components leading to more computational power and smaller sensing devices. One class of materials capable to fulfil this role is the class of 2D materials.

The major discovery igniting the field of 2D materials, now almost fifteen years ago, was made by Geim and Novoselov.¹ Atomically thin layers of graphite were isolated. A modest number of additional atomic thin 2D materials were discovered after graphene ranging from conductors (graphene) to semiconductors (phosphorene) to insulators (hexagonal boron-nitride). The possibility to assemble electric devices by stacking different monolayers called van der Waals heterostructures, unlocks a vast number of possible device structures utilizing the different characteristics of the 2D building blocks.

The aim of this work is to complement the world of atomically thin materials with 2D-triazine based graphitic carbon nitride (TGCN). TGCN carries interesting properties like a bandgap of 1.8 eV and good electrochemical stability. The nitrogen sites add intriguing possibilities to dope TGCN or to use their properties for conductometric sensing.

The experimental goals are to synthesize large crystalline TGCN films from which monolayers can be isolated for the first time, marking the birth of TGCN as 2D material. Devices produced based on these monolayers will elucidate the optical, electronic and mechanical characteristics of this new 2D material.

Supported by European Research Council (ERC) under the Starting Grant scheme (BEGMAT – 678462).

1. Novoselov, K. S. et al., *Science* **2004**, 5696, 666-669, DOI: 10.1126/science.1102896.
2. Algara-Siller et al., *G. Angewandte Chemie* **2014**, 29 7450-7455, DOI: 10.1002/anie.201402191.



Intra- and intermolecular charge transfer in the optical excitations of J-aggregates formed by push-pull chromophores

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^cDipartimento di Scienze Chimiche, Università di Padova, 35131 Padova, IT

The microscopic nature of optical excitations in J-aggregates, a peculiar class of organic crystals exhibiting enhanced light-matter interaction, is still far from being properly understood. In a first-principles study based on density-functional theory and many-body perturbation theory, we analyze a J-aggregate composed of push-pull dyes. While previous work showed the supramolecular character of the excitations in the J-band¹, here we unravel the interplay between intra- and inter-molecular charge transfer (CT) in terms of exciton wavefunction analysis. Our first-principles results demonstrate the coexistence between excited states with mixed intra- and inter-molecular CT with states with pure intermolecular CT.² Since the latter are associated with very low absorption, they cannot be detected in conventional absorption experiments. Our findings offer new perspectives to further understand the nature of collective excitations in organic semiconductors.

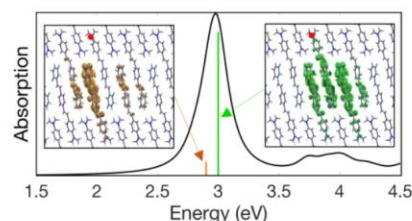


Figure 1. First-principles optical absorption spectrum of J-aggregate composed of push-pull dyes. In the insets are reported the excitons isosurfaces corresponding to two representative excited states within the J-band: a pure intermolecular charge-transfer exciton (brown) and a mixed inter- and intra-molecular charge-transfer excitons.

Supported by the European Union under the ERC grant TAME Plasmons (project number ERC-CoG-681285), by the Deutsche Forschungsgemeinschaft (Projektnummer 182087777 - SFB 951 and HE 5866/2-1), and by the EU Centre of Excellence "MaX - Materials Design at the Exascale" (Horizon 2020 EINFRA-5, Grant No. 676598). M.G. acknowledges support from the German Academic Exchange Service (DAAD) and HPCEUROPA3 (INFRAIA-2016-1-730897). Computational resources were partly provided by PRACE on the Marconi machine at CINECA and by the High-Performance Computing Center Stuttgart (HLRS)

¹ M. Guerrini, A. Calzolari, and S. Corni, *ACS Omega*, **3**, 10481. (2018)

² M. Guerrini, C. Cocchi; D. Varsano, A. Calzolari, S. Corni *J. Phys. Chem C*, **2019**, 123, 11, 6831-6838



Fully aromatic, covalent phosphinine frameworks: from synthesis to application

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^aDepartment of Chemistry, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489, Berlin, D

Structural modularity of polymer frameworks is a vital advantage of covalent organic polymers, however, only C, N, O and S have found their way into their π -conjugated aromatic building blocks so far.^{1,2} Here, we expand the toolbox available to polymer and materials chemists by one additional nonmetal, phosphorus. Starting with a building block that contains a λ_5 -phosphinine (C_5P) moiety, we evaluate a number of polymerization protocols, finally obtaining fully aromatic, covalent phosphinine-based frameworks (CPFs) via Suzuki-Miyaura coupling (CPF-1) or Stille-coupling. CPFs are all porous polymer glass with extremely high thermal stability. Among CPFs, CPF-1 is a weakly porous polymer glass ($72.4 \text{ m}^2 \text{ g}^{-1} \text{ N}_2 \text{ BET at } 77 \text{ K}$) with green fluorescence ($\lambda_{\text{max}} 546 \text{ nm}$). CPF-1 catalyzes hydrogen evolution from water under UV and visible light irradiation without the need for additional co-catalyst at a rate of $33.3 \mu\text{mol h}^{-1} \text{ g}^{-1}$. Our results demonstrate for the first time the incorporation of the phosphinine motif into complex polymer frameworks since the first phosphinine compound was synthesized in 1966.³ Phosphinine-based frameworks show promising electronic and optical properties that might spark future interest in their applications in light-emitting devices and heterogeneous catalysis.

Supported by European Research Council (ERC) under the Starting Grant scheme (BEGMAT – 678462).

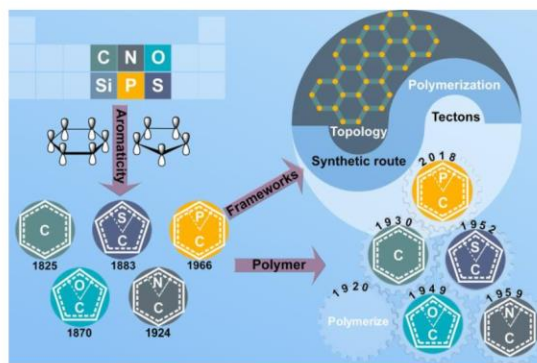


Figure 1. Progress of covalent phosphinine frameworks

¹ D. Schwarz et. al, *Chem. Eur. J.* **2018**, 24 (46), 11916. DOI: 10.1002/chem.201802902

² Y. S. Kochergin et. al, *Angew. Chem.* **2018**, 57(43), 14188. DOI: 10.1002/anie.201809702

³ G. Märkl, *Angew. Chem.* **1966**, 5(9), 846. DOI: 10.1002/anie.196608463



Producing impactful science: general guidelines for day to day research

Margherita Citroni, *Nature Communications*, Heidelberger Platz 3, 14197 Berlin, Germany

Good research is the foundation of impactful science, but how does every day work translate into influential output? In this talk we will discuss and define what impact is and what Nature Research editors look for in potential publications. I will review recent Nature journal articles in the field of materials chemistry (published in *Nature*, *Nature Materials*, *Nature Nanotechnology* and *Nature Communications*), and highlight the reasons for why they were considered potentially impactful.

In addition, we'll assess whether there are ways to tweak day to day research towards impactful results. Finally, I will discuss ongoing initiatives at the Nature journals that are designed to encourage open research, including data availability and sharing.

Margherita Citroni is an Associate Editor at *Nature Communications*, where she handles content in physical, analytical and materials chemistry. Before becoming a full-time editor, Margherita was a researcher at the European Laboratory for Non Linear Spectroscopy in Florence, Italy, where she studied chemical reactivity and phase transitions in molecular systems under extreme pressures.



An illuminating perspective on nanomaterials from *ab initio* electronic structure theory

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The progressing advances towards the production of nanomaterials and the manipulation of their properties down to the atomistic scale call for reliable theoretical approaches that are able to support and rationalize the experimental observations. *Ab initio* methods for electronic-structure theory are perfectly suited for these tasks, as they can describe quantum-mechanically the structural, electronic, and optical properties of ideally any material without the prior knowledge of any empirical parameters. In this talk, I will give an overview on the *ab initio* methods based on (time-dependent) density-functional theory that are employed in our group to investigate light-matter interaction. With selected examples from our recent work on the femtosecond dynamics of organic and hybrid materials^{1,2} (see Fig. 1), I will illustrate the capability of these methods to represent, predict, and understand the phenomena related to the interaction of electromagnetic fields up to the ultrafast time domain.

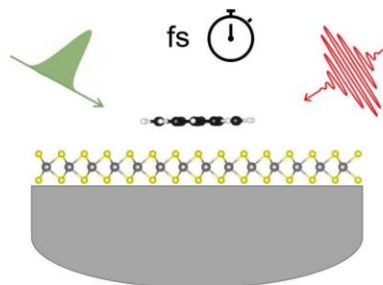


Figure 1. Pictorial representation of the setup for simulations of pump-probe experiments in the ultrafast time scale.

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Computational time provided by the Norddeutscher Verbund für Hoch- und Höchstleistungsrechnen (HLRN).

¹ J. Krumland et al., *in preparation*

² M. Jacobs et al., *in preparation*



Low-cost carbon nanofiber textiles as free-standing electrodes in supercapacitors

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The development of renewable energy sources and the recent advances in portable electronics boosts the development of energy storage devices amongst which batteries and electrochemical capacitors (ECs) play a major and complementary role. Electrochemical supercapacitors provide higher power density than Li-ion batteries (~ 15 kW/kg vs ~ 0.35 kW/kg) but less energy density (~ 15 W.h/kg vs ~ 260 W.h/kg). Recently, the coming generation of portable devices has been even more demanding in terms of material requirements, thus aiming for cheap and highly dense electrodes produced from widely available materials.

Herein, we present the production of high-density carbon nanofiber electrodes and their performance in aqueous supercapacitors. We electrospin in a controlled environment an alkaline solution of organosolv lignin (OSL) blended with 10% PEO and press the obtained mat at 40 bar to obtain a dense but porous structure. Due to the low pore tortuosity and the absence of binder, the electrodes show high electrical conductivities up to 5 S/cm and a high capacitance retention over 80% at 100 A/g. The electrodes show a volumetric capacitance of 130 F/cm³ which is one of the highest volumetric values reported for biomass related precursors.

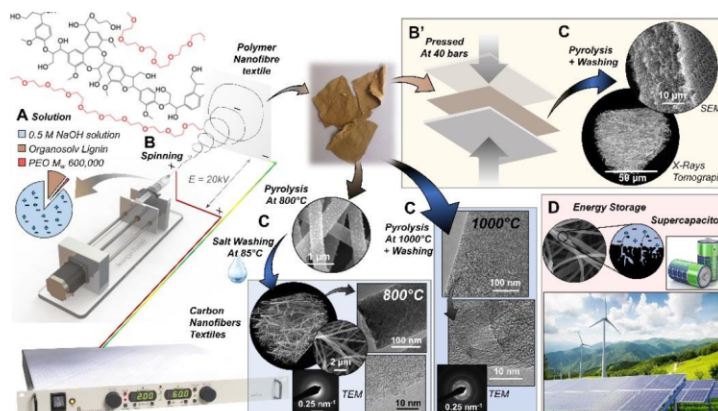


Figure 1. Overview of the carbon nanofibre textile synthesis and their application as electrodes in supercapacitors



Block copolymer template-directed synthesis of well-ordered composite nanostructures

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3D nanostructured organic@inorganic composite materials are considered as promising candidates for various practical applications, such as catalysis or energy storage materials. Compared to common approaches, such as de-alloying and sol-gel synthesis¹, block copolymers (BCP) have the ability to self-assemble into highly ordered porous nanostructures that can be applied as soft templates for the preparation of well-ordered inorganic or organic@inorganic composite materials².

In our study, a selective swelling process will induce porous structures of the PS-P2VP nanospheres. Porous TiO_2 particles with interconnected pore structures have been developed by using porous PS-P2VP particles as template as shown in Fig.1, which can be applied as a new type of sulfur-host material for lithium-sulfur batteries³. In order to improve the conductivity of the obtained particles, a thin layer of carbon has been coated on the surface. The thin carbon layer induces better contact between the TiO_2 particles and the carbon black of the slurry without disturbing the chemical confinement of polysulfides by TiO_2 . Enhanced capacity with better cycling stability has been observed for the carbon-coated TiO_2 particles-based cathode materials.

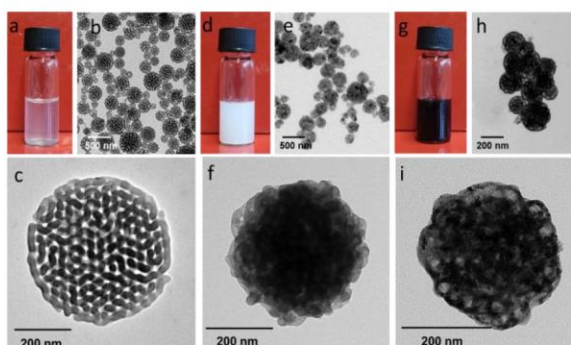


Figure 1. Photos of the porous PS-P2VP particles (a), TiO_2 @PS-P2VP particles (d) and TiO_2 particles (g) dispersed in ethanol. TEM images of the porous PS-P2VP particles (b, c), TiO_2 @PS-P2VP particles (e, f), and porous TiO_2 particles (h, i).

¹ I. Vukovic, G. ten Brinke, K. Loos, *Polymer*, **2013**, 54, 2591–2605.

² S. Mei, J. Cao, Y. Lu, *J. Mater. Chem. A*, **2015**, 3, 3382 – 3389.

³ S. Mei, C. J. Jafra, I. Lauermann, Q. Ran, M. Kärger, M. Ballauff, Y. Lu, *Adv. Funct. Mater.* **2017**, 26, 1701176.



Generating fully heterocyclic and aromatic materials hydrothermally

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Organic materials' position in the materials space is mainly characterized through a combination of low specific weight with a large range of chemical functionalities. The latter is enabled through the many possible moieties that can be generated by carbon and heteroatoms. When organic moieties contain a large amount of double and triple bonds, and even more so when these are conjugated, impressive thermal stabilities of > 500 °C arise additionally. Hence, the highest possible thermal stabilities in organic materials are found at an exclusively aromatic, heteroaromatic, and heterocyclic build-up. Synthesizing such materials involves harsh, environmentally harmful, and toxic procedures by the vast majority of routes. We have recently developed fully hydrothermal syntheses (HTS) for such materials. With this presentation, I will show that HTS can be employed for a wide range of materials classes (e.g. polymers, pigments, and dyes) and molecular dimensions and connectivities (*i.e.* small molecules, linear polymers, networks and frameworks). Most intriguingly, HTS generates improved materials properties as compared to classical routes. This is a consequence of HTS often generating crystalline over amorphous products. Moreover, I will present our efforts to transfer these HTS procedures back to society, including industrial implementation and education.

Supported by the Austrian Science Fund (FWF) under the Grant "HYDROCOF – The hydrothermal route to covalent organic frameworks" (START Y1037-N28), the Austrian Science Fund (FWF) and the Christian-Doppler Society (CDG) under the Grant "Polyimide-Reinforced High-Performance Composites" (PIR 10-N28), the Vienna Science and Technology Fund (WWTF) under the Grant "3C- Cellular Color Chart" (LS17-051), and the aws (Austria Wirtschaftsservice) under the prototype Grant "Hochleistungsmembranen" (1504501).



Polyimide processing from aqueous solutions

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Polyimide (PIs) are of great relevance in modern technology as they are one of the most important materials used in electronics for insulating electrically conducting parts. PIs' use in electronic devices is based on their materials properties: they feature low dielectric constants, high thermal and mechanical stability, and low specific weight.¹ In insulating applications, PIs are used as films, *i.e.* conductors are covered with a thin layer of a PI. Since PIs are thermosets once fully cured, PI films have to be generated from a prepolymer solution, *i.e.* a poly(amic acid, PAA) solution in an aprotic polar solvent such as *N*-methylpyrrolidone (NMP).² PAA solutions are applied as coatings and cured to the PIs through several heating steps. These processing conditions are very expensive, but more importantly the use of the required solvents by electronic manufacturers is expected to be forbidden in the coming years. NMP for instance is already on the so-called "REACH watchlist".³ Therefore, electronics manufacturers are heavily seeking green alternatives for PI processing. We here present our results in generating PI films from aqueous solutions.⁴ With this contribution, we discuss (*i*) our molecular design approach for rendering monomers water-soluble, (*ii*) the film formation processes, and (*iii*) the materials properties of the obtained films.

This work is supported by the aws (Austria Wirtschaftsservice) prototype grant "AQPolyimide-Polyimidherstellung und -Verarbeitung aus wässriger Lösung" (P1621609).

¹ W. Volksen et. al, *Chem. Rev.* **2010**, *110*, 56. DOI: 10.1021/cr9002819

² P. M. Hergenrother et. al, *High. Perform. Polym.* **2003**, *15*, 3. DOI: 10.1177/095400830301500101

³ Registration, Evaluation, Authorisation and Restriction of Chemicals, Regulation EC 1907/2006

⁴ S. España-Orozco and Miriam M. Unterlass, *Verfahren zur Herstellung von Polyimiden* Patent application: At A 383/2016; submitted on August 19, 2016.



Olefin-linked covalent organic frameworks (COFs)

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Two-dimensional (2D) covalent organic frameworks (COFs) have emerged as a promising class of materials for various applications such as gas storage and separation, energy storage, photovoltaics, (opto)-electronics, ion conduction and heterogeneous catalysis.¹ The extended 2D π -conjugation combined with their high surface area and porosity make these materials also attractive for photocatalytic applications.^{2,3} The crystallization of such extended COFs is achieved by reticulating rigid organic building blocks through reversible B-O, B-N, Si-O, C-N bond formation reactions.^{4,5} Recently, the development of cyanovinylene linked COFs have for the first time applied an olefin ($-C=C-$) linkage for the crystallization of extended crystalline COFs, albeit just very few examples have been achieved so far.^{6,7}

Herein, we report a new strategy for the crystallization entirely olefin ($-C=C-$) linked 2D COFs (V-COFs). V-COFs are crystalline and exhibits permanent porosity and a surface area ranging from 630 m²/g to 1341 m²/g. The high chemical stability combined with a fully π -conjugated backbone and abundant nitrogen atoms within the framework make V-COFs promising materials in heterogeneous catalysis.

¹ S.-Y. Ding et. al, *Chem. Soc. Rev.* **2013**, 42, 548–568.

² P. Pachfule, et. al, *J. Am. Chem. Soc.* **2018**, 140, 1423–1427.

³ T. Banerjee, et. al, *ACS Energy Lett.* **2018**, 3, 400–409.

⁴ P. J. Waller, et. al, *Acc. Chem. Res.* **2015**, 48, 3053–3063.

⁵ J. Roeser, et. al, *Nat. Chem.* **2017**, 9, 977–982.

⁶ E. Jin, et. al, *Science*. **2017**, 357, 673–676.

⁷ X. Zhuang, et. al, *Polym. Chem.* **2016**, 7, 4176–4181.



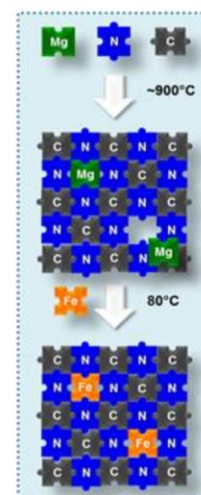
Active-site imprinting towards tailored carbon electrocatalysts

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Atomically dispersed catalysts are a class of materials that sparked a lot of interest, since analytical tools with atomic resolution are widely available. One class of such catalysts, so-called iron-coordinated nitrogen doped carbons (Fe-N-Cs), are considered the most promising non-noble alternatives for Pt-based catalysts for the oxygen reduction reaction (ORR) in PEM fuel cells.^{1, 2, 3} The preparation is believed to require harsh reaction conditions that complicate the selective formation of the square-planar FeN₄ active sites.⁴ We recently introduced a mild procedure, which leads to active-site formation at low temperatures in a wet-chemical coordination step, essentially by decoupling the carbonization from the preparation of the active sites.⁵

The key concept herein is the so-called active-site imprinting into the NC before the involvement of the active transition metal. Lewis basic Mg²⁺ ions, just like Fe²⁺ ions, support square-planar coordination with four nitrogens (as observed in chlorophyll), however it is thermodynamically more stable towards side reactions at high temperatures. Hence, Mg²⁺ can be exploited to imprint N₄ sites into NCs, that can later be exchanged with Fe ions to obtain for example active ORR catalysts (see Figure). Other metal ions, such as Zn²⁺, are also interesting template ions for that purpose. While Zn²⁺ is more likely to show side reactions at high temperatures, there are numerous preparation procedures of NCs prepared in the presence of Zn²⁺ available. In this presentation I will discuss our recent results in this direction and present different aspects of Zn²⁺ coordination to NCs and the derived Fe-N-C catalysts in the context of ORR electrocatalysis.



¹ M. Lefèvre, E. Proietti, F. Jaouen, J.-P. Dodelet, Science, 324 (2009) 71-74.

² G Wu, KL More, CM Johnston, P Zelenay, Science 332 (6028), 443-447.

³ H. A. Gasteiger, S. S. Kocha, B. Sompalli, F. T. Wagner, Applied Catalysis B, 56, (2005), 1-2, 9-35.

⁴ S. Gupta, D. Tryk, I. Bae, W. Aldred and E. Yeager, J. Appl. Electrochem., 19, (1989), 19-27.

⁵ A. Mehmood, J. Pampel, G. Ali, H. Y. Ha, F. Ruiz-Zepeda, and T.-P. Fellerger, Adv. Energy Mater. 2017), 1701771.



Composite of spinel NiFe_2O_4 and heteroatom doped carbon fibre derived from lignin as bifunctional oxygen electrocatalyst

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Bifunctional electrocatalyst is the key component of regenerative fuel cells and metal-air batteries. However, material development is hindered by naturally sluggish kinetics of oxygen catalysis. Heteroatom doped carbon has been proven to be active for oxygen reduction reaction (ORR)¹ while binary transition metal oxide (TMO) are well-known for their ability to evolve oxygen (OER).² The idea of fabricating composite of metal oxide and heteroatom doped carbon nanofibre (TMO/NP-CNF) derived from lignin is to utilize synergetic effect for both chemical reactions, ORR and OER, on a single free-standing material, where NP-CNF can also serve as a charge-transport media.

Nitrogen and phosphorus doped carbon fibres (NP-CNF) were electrospun from lignin solution added melamine and/or ADP as a single or various doping sources. The synthesis approach has manifested our effort to exploit unveiled values of industrial by-products, particularly kraft lignin from pulping in this case. Ni-Fe compound nanoparticles achieved by hydrothermal were intercalated into carbon fibre via coaxial electrospinning.

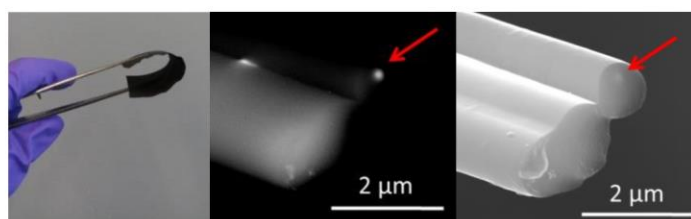


Figure 1. a) The flexible carbon mat, b) BSE image of the composite and its according SE image, red arrow shows the particle inside the fibre

¹ Rao, C. V.; Cabrera, C R.; Ishikawa, Y., *The Journal of Physical Chemistry Letters* **2010**, 1 (18), 2622-2627. DOI: 10.1021/jz100971v

² Hong, W. T.; Risch, M.; Stoerzinger, K. A.; Grimaud, A.; Suntivich, J.; Shao-Horn, Y., *Energy & Environmental Science* **2015**, 8 (5), 1404-1427. DOI: 10.1039/C4EE03869J



Superhydrophobic materials fabrication using polymer-nanoparticle composites

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Highly water repellent materials are a class of functional material which show great promise industrially and commercially, due to the inherent properties they possess. These materials have such a low affinity for water that upon contact, water droplets bead into near-spherical droplets, and roll easily across these surfaces (Fig. 1a). The potential applications for these materials include; self-cleaning ('Lotus Effect'), anti-biofouling and drag reduction, in addition to others.¹ Engineering nano- and micro-surface structures from inorganic nanoparticles, followed by post treatment with an organic coating (molecular or polymeric) is an inexpensive and commonly used fabrication route to generate superhydrophobic nanomaterials.^{2,3} However, artificial superhydrophobic materials often face environmental challenges due to their weak mechanical strength and susceptibility to UV degradation which inhibit their widespread use. The presented work will detail a general fabrication approach to generating superhydrophobic polymer-nanoparticle composites using solution based formulations and a solvent free approach. We discuss how we can tune the polymer:nanoparticle ratio i.e. the average thickness of the polymer coating surrounding nanoparticles (r_{poly}) (Fig.1b) and show the impact this has on overall functionality. Furthermore, we show how the mechanical strength of films can be improved by incorporating an adhesive and assess the enhanced UV durability of polymer composite materials in comparison to molecular functionalisation, increasing the real-world applicability of these functional materials.

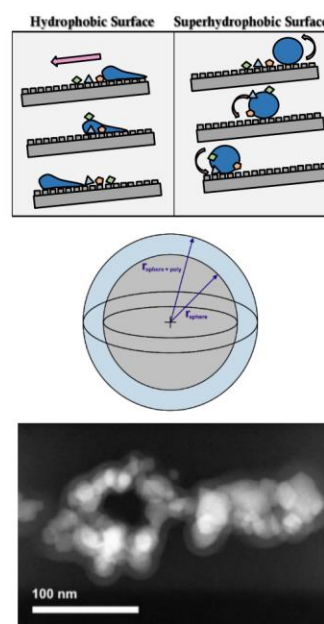


Figure 1. (a) self-cleaning mechanism of hydrophobic surfaces vs superhydrophobic surfaces; (b) structure of nanoparticle-polymer composite; and (c) scanning transmission electron microscopy image of composite material.

¹W. Barthlott et. al, *Planta*, **1997**, 202, 1–8.

DOI:10.1007/s004250050096

²H. J. Perera et. al, *J. Appl. Polym. Sci.*, **2016**, 133. DOI: 10.1002/app.44072

³L. Xu et. al, *ACS Appl. Mater. Interfaces*, **2012**, 4, 1118–1125. DOI: 10.1021/am201750h



Nonaqueous synthesis of Nb₂O₅@carbon nanoparticles and nanospheres for high performance hybrid supercapacitors

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Hybrid supercapacitors (HSCs) consist of a high-capacity ion (e.g. Li⁺ or Na⁺) battery type electrode as anode and high-rate capacitive electrochemical double layer capacitance (EDLC) type electrode as cathode, and are considered as promising electrical energy storage devices, due to their simultaneous high energy density and power density.¹ However, the development of high-performance HSCs is restricted by the sluggish faradaic ion intercalation at the anode. High rate pseudocapacitive oxides are good candidates for the anode of HSCs.² Among those, orthorhombic Nb₂O₅ is attractive due to its high theoretical capacity (~200 mAh g⁻¹), fast ion (Li⁺ or Na⁺) diffusion and excellent energy storage. However, the electrical conductivity of Nb₂O₅ is poor, nanoparticles tend to agglomerate, making it difficult to disperse and mix them with conductive additives, and nanostructured materials can easily collapse or sinter at the high temperatures (600-800 °C) needed to form T-Nb₂O₅.³

In this work, small orthorhombic niobium oxide nanoparticles wrapped with carbon (T-Nb₂O₅@C NP) were synthesized in a two-step process. The organics formed in situ are homogeneously bound to the surface of the nanoparticles, which allows the formation of a homogenous carbon coating while preventing a significant growth and agglomeration of the nanoparticles. Hybrid supercapacitors (HSCs), including both Li-HSCs and Na-HSCs, were assembled by using the T-Nb₂O₅@C samples as anode and a commercial activated carbon (YPF-50, Kuraray) as cathode in an organic electrolyte. The T-Nb₂O₅@C NPs with 10 wt.% carbon showed high reversible rate capacity within a voltage range from 3.0 to 1.0 V (vs Li/Li⁺). The assembled Li-HSCs of this sample showed very high energy density and power density, and stable cycling performance. In addition, for the Na-HSCs, both of T-Nb₂O₅@C NPs and NSs with 15 wt. % carbon showed good reversible capacity within a voltage range from 3.0 to 0.01 V (vs Na/Na⁺).

¹ H.W. Wang et. al, *Advanced Materials* **2017**, 29, 1702093. DOI: 10.1002/adma.201702093

² V. Augustyn et. al, *Energy & Environmental Science* **2014**, 7, 1597. DOI:10.1039/C3EE44164D

³ V. Augustyn et. al, *Nat Mater* **2013**, 12, 518. DOI: 10.1038/nmat3601



All-cellulose-based quasi-solid-state sodium-ion hybrid capacitors enabled by structural hierarchy

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Na-ion hybrid capacitors consisting of battery-type anodes and capacitor-style cathodes are attracting increasing attention on account of the abundance of sodium-based resources as well as the potential to bridge the gap between batteries (high energy density) and supercapacitors (high power). Cellulose is the most available and renewable resource in nature.

Herein, hierarchically structured carbon materials inspired by the multiscale building units of cellulose in nature were assembled with a cellulose-based gel electrolyte into a Na-ion capacitor. The nonporous hard carbon anodes were obtained through direct thermal pyrolysis of cellulose nanocrystals. Nitrogen-doped carbon cathodes with a coral-like

hierarchically porous architecture were prepared via hydrothermal carbonisation and activation of cellulose microfibrils. The reversible charge capacity of anode is 256.9 mA h g⁻¹ when operating at the current density of 0.1 A g⁻¹ (from 0–1.5 V vs. Na⁺/Na), and the discharge capacitance of cathodes tested in half cells (within 1.5–4.2 V vs. Na⁺/Na) is 212.4 F g⁻¹ at the same current density. Utilizing Na⁺ and ClO₄⁻ as charge carriers, the energy density of the full Na-ion capacitors with two asymmetric carbon electrodes can reach 181 W h kg⁻¹ at 250 W kg⁻¹, which is one of the highest energy devices reported until now. Combined with a hydroxyethyl cellulose-based gel electrolyte, an all-cellulose-based quasi-solid-state device was demonstrated with possessing additional advantages in terms of precursors costs and overall sustainability.

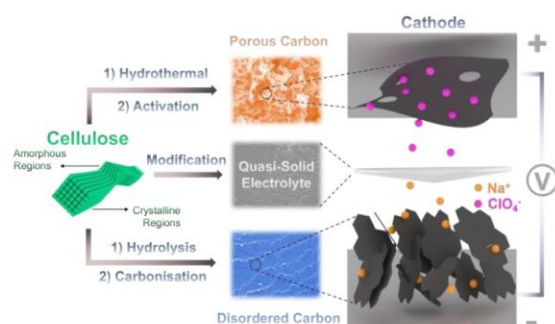


Figure 1. Schematic diagram illustrating the 'one-for-all' synthesis processes of electrodes and electrolytes as well as the asymmetric configuration of NICs.

Supported by the CSC scholarship (201706630019), EPSRC (EP/R021554/1, EP/S018204/1).

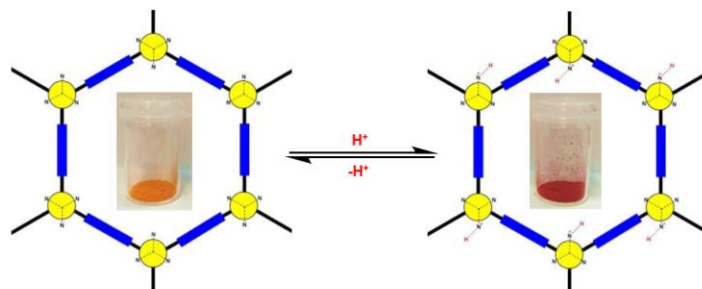


A real-time optical and electronic chemical sensor based on triazine-containing 2D materials

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Fully-aromatic, two-dimensional covalent organic frameworks (2D COFs) are hailed as candidates for electronic and optical devices, yet to-date few applications emerged that make genuine use of their rational, predictive design principles and permanent pore structure. In the last decade, triazine containing covalent organic frameworks/polymers has been extensively studied in photocatalysis and as a semiconductor.^{1 2 3} Although photocatalytic activity of these materials is discussed in terms of the band gap energy, the efforts to modulate or reversibly tune the optical band gap demands more study. Here, we present some examples of 2D COFs, which exhibits a dramatic real-time response in the visible spectrum and an increase in bulk conductivity by several orders of magnitude to a chemical trigger - corrosive HCl vapours. The optical and electronic response is fully reversible using a chemical switch (NH₃ vapours) or physical triggers (temperature or vacuum). These findings demonstrate a useful application of fully-aromatic 2D COFs as real-time responsive chemosensors and switches.



Supported by European Research Council (ERC) under the Starting Grant scheme (BEGMAT – 678462).

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² Y. S. Kochergin et. al, *Angew. Chem.* **2018**, 57(43), 14188. DOI: 10.1002/anie.201809702

³ M.J. Bojdys et. al, *Angew. Chem.* **2014**, 53, 87450. DOI:10.1002/anie.201482971



Sustainable is the new black

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One of the grand challenges facing humanity today is access to sustainable materials and chemicals which are at the heart of sustainable technologies. The production of materials, chemicals and fuels from abundant and renewable resources will eliminate our dependence on petroleum/critical metal-based supplies and will provide access to a new economy based on available reserves. Carbon is the most versatile element known. It combines with other (carbon) atoms giving rise to new carbon materials with astonishing properties. The versatility and potential of carbon has attracted top recognition in the last decade for the work in fullerenes (1996 Nobel Prize in Chemistry), CNTs (2008 Kavli Prize in Nanoscience) and grapheme (2010 Nobel Prize in Physics). However, the mystery and wonder of carbon offers more to discover.

While carbon is widespread on Earth, it has been mainly synthesized from fossil fuel-based precursors with sophisticated and energy consuming methodologies that generate toxic gases and chemicals. The preparation of carbon materials from renewable resources is a key research challenge in terms of sustainability, climate change and economics. Since the beginning Nature created carbon from biomass.

We have demonstrated that it is possible to mimicking the natural process of carbon formation and prepare carbon nanomaterials from biomass using mild hydrothermal processes. Along with amorphous carbon materials (denoted HTC), this procedure also enables biomass transformation into useful chemicals such as 5-hydroxymethylfurfural (5-HMF) or levulinic acid (LA). Recently, we have discovered a third product of Hydrothermal Carbonisation - a crystalline form of carbon - arising at the interface between the amorphous HTC microspheres and the aqueous phase containing the biomass-derived chemicals.

In this talk I will present some of the fundamentals governing the production of carbon nanomaterials and chemicals. We will also discuss the application of HTC materials in electrocatalytic reactions such as Oxygen Reduction Reaction as well as for energy storage in Na-ion batteries and supercapacitors.

Finally, some of the photo-physics governing the optoelectronic properties of the new family of fluorescent hydrothermal carbon nanocrystals will be presented.



Polyglycerol based broadly active multivalent inhibitors of influenza virus

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Half a million deaths and 3-5 million cases of severe illness per year, and high mutation frequency push the constant need for developing new therapeutics against influenza virus infection. Two glycoproteins hemagglutinin (HA) and neuraminidase (NA) are responsible for the influenza virus attachment to the cell and then the release of progeny virus particles from the infected cell surface respectively. Abundant HA protein on the Influenza virus surface multivalently binds with the exposed sialosides on the cell surface leading to the cellular entry of virus particles. Influenza virus inhibition in the early stages of infection by multivalent sialosides requires an optimized ligand geometry with an appropriate multivalent ligand presentation. Architectural requirements and optimal ligand densities were identified for an efficient inhibitor of influenza A virus (X31/H3N2). Linear and dendritic polyglycerol sialosides with similar molecular weights and chemical constructs were compared achieving low nanomolar inhibitors of influenza A virus (X31/H3N2). *In vivo* application clearly confirms the high inhibition potential of the optimized linear candidate over the dendritic one without any acute toxicity. Further development of NA and the mix inhibitors clearly shows the broad antiviral activity within low nanomolar concentration in the later stages of infection.

Supported by the SFB 765

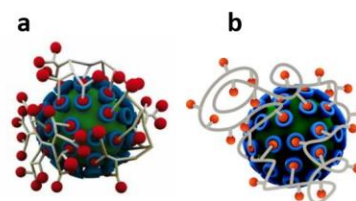


Figure 1. a) Dendritic and b) linear architectures with similar molecular weight decorated with ligands (red) effectively bind and shield the virus surface.

1. Sumati Bhatia, et al. *Journal of American Chemical Society* **2016**, 138, 8654–8666.
2. Sumati Bhatia, et al., *Biomaterials* **2017**, 138, 22-34.
3. Mammen et al., *Angew. Chem. Int. Ed.* **1998**, 37, 2754-2794.



Synthesis of high-performance covalent organic frameworks *via* a green hydrothermal route

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High-performance materials (HPMs) syntheses are to date mostly harmful to the environment and human health, energy-intensive, and require solvents derived from petrol, which is a depleting resource. One way to develop green and innovative pathways to HPMs is to take inspiration from chemical processes in nature. We recently developed a novel and green route for synthesizing heterocycle-linked organic HPMs, using nothing but high-temperature water as reaction medium: hydrothermal polymerization (HTP)¹. HTP is a geomimetic approach inspired by the natural mineral formation process “*hydrothermal crystallization*”, by which highly crystalline networks such as quartz form within hydrothermal veins. As its natural counterpart, HTP generates high crystallinity in organic materials².

The majority of covalent organic frameworks (COFs) reported to date disintegrate relatively easily under hydrolytic strain. Therefore, high-performance COFs linked by strong heterocyclic functions have recently attracted considerable interest.³ However, the latter are hard to obtain: generating crystallinity in COFs requires rendering the linking functions reversible under reaction conditions for correcting errors arising from kinetic attachment. As we have shown that crystalline heterocycle-linked organic materials can be obtained hydrothermally,² we believe that HTP bears unique potential for generating high-performance COFs. With this contribution, we explore the formation of COFs via HTP including the discussion of a thorough set of characterizations of the obtained HPMs by various techniques.

Supported by the Austrian Science Fund (FWF) under the Grant “HYDROCOF – The hydrothermal route to covalent organic frameworks” (START Y1037-N28)

¹ B. Baumgartner et. al, *Polymer Chemistry* **2014**, 5, 3771. DOI: 10.1039/C4PY00263F

² M. M. Unterlass, *Angew. Chem. Int. Ed.* **2018**, 57, 2292. DOI: 10.1002/anie.201713359

³ C. R. DeBlase et. al, *Macromolecules* **2016**, 49, 5297. DOI: 10.1021/acs.macromol.6b00891



Ladder polymers for hydrogen evolution from water

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The clean, sustainable production of hydrogen is one promising strategy for future zero-emission energy supply.¹ Conjugated linear polymers containing dibenzo[*b,d*]thiophene sulfone units have been shown repeatedly to outperform most other organic photocatalysts for hydrogen evolution from water under sacrificial conditions.² Here, we present the combination of structural features derived from highly active linear polymer

photocatalysts with the increased conjugation that might be expected for a conjugated ladder polymer. Starting from a linear conjugated polymer (**cLiP1**), two ladder polymers were synthesized via postpolymerization annulation and oxidation techniques to generate rigidified, planarized materials bearing dibenzo[*b,d*]thiophene (**cLaP1**) and dibenzo[*b,d*]thiophene sulfone subunits (**cLaP2**).³ The high photocatalytic activity of **cLaP1** (1307 $\mu\text{mol h}^{-1} \text{g}^{-1}$) in comparison to **cLaP2** (18 $\mu\text{mol h}^{-1} \text{g}^{-1}$) under broadband illumination ($\lambda > 295 \text{ nm}$) in presence of a hole-scavenger was attributed to a higher yield of long-lived charges (μs – ms timescale), as evidenced by transient absorption spectroscopy. Additionally, **cLaP1** has a larger overpotential for proton reduction and thus an increased driving force for the evolution of hydrogen under sacrificial conditions.

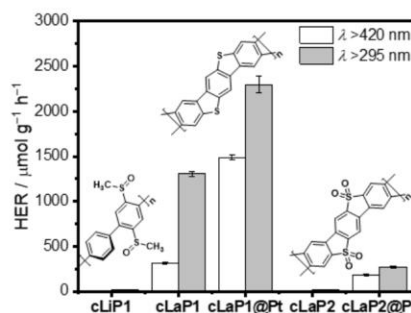


Figure 1. Hydrogen evolution rates comparison for a series of conjugated polymers.

This project has received funding from the European Union's Horizon 2020 research and innovation programme (Marie-Sklodowska-Curie Individual Fellowship to AV) under grant agreement No 796322.

¹ P. P. Edwards et al, *Energy Policy*, **2008**, 36, 4356–4362.

² a) R. S. Sprick et al, *Angew. Chem. Int. Ed.*, **2016**, 55, 1792–1796; b) X. Wang et al, *Nat. Chem.*, **2018**, 10, 1180–1189; c) Z. Wang et al, *ACS Catal.*, **2018**, 8, 8590–8596; d) C. Dai et al, *Small*, **2018**, 14, 1801839; e) M. Sachs et al, *Nat. Commun.*, **2018**, 9, 4968.

³ A. Vogel et al, *Faraday Discuss.*, **2018**; DOI: 10.1039/C8FD00197A.



Tailor-made carbazole-based microporous polymer networks for photocatalytic applications

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Microporous Polymer Networks (MPNs) are an emerging class of functional materials, which show exceptionally high porosity, as well as thermal and chemical stability. Since these networks consist of purely organic building units, the chemical nature of large accessible surface areas are controllable to obtain the desired physical properties. By tailoring the material properties in a controlled fashion, MPNs exhibit the potential for a broad range of applications, including gas storage, heterogeneous catalysis and energy storage devices.^[1,2,3]

Herein, we present carbazole-based microporous networks synthesized *via* oxidative polymerization, especially tailor-made for (photo)catalytic applications. For this purpose, polymers bearing bipyridinyl chelating functionalities were constructed and coordinated with rhenium species [Re(bipy)(CO)₄], to photocatalyze the reduction of carbon dioxide to carbon monoxide. By means of visible-light irradiation carbon monoxide evolution rates up to 623 $\mu\text{mol g}^{-1} \text{h}^{-1}$ in 97.8% selectivity are obtained.^[4] In order to improve the photocatalytic performance in MPNs, we have designed further photocatalytic systems to control the porous characteristics, morphology and spatial distribution of the functional groups within the MPNs.

DFG (1463/15-1), Chinesisch-Deutsches Zentrum für Wissenschaftsförderung (GZ1286)

¹ Q. Chen, M. Luo, P. Hammershøj, D. Zhou, Y. Han, V. Wegge Laursen, C. Yan, B.-H. Han, *J. Am. Chem. Soc.* **2012**, 134, 6084–6087. DOI: 10.1021/ja300438w

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³ H. Liang, Y. Chen, B.-H. Han, *ACS Catal.* **2018**, 8, 5313–5322. DOI: 10.1021/acscatal.7b04494

⁴ H. Liang, S. Vogl, A. Acharjya, D. Assefa, T. Wang, Q. Chen, A. Thomas, B.-H. Han, *ACS Catal.*, **2019**, manuscript just accepted. DOI: 10.1021/acscatal.8b04032



Lignin-derived electrospun freestanding carbons as alternative electrodes for RFB

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Carbon-based flexible fibre mats have been electrospun from a sustainable biomass source (Figure 1a). Through the synthesis and post-treatment, properties such as the porosity, surface area and doping of the fibres were tuned (Figure 1 e-i). These modifications have a direct influence on their performance as free-standing electrodes for vanadium redox flow batteries (VRFB). The morphology of the electrodes has been characterised through X-ray computed tomography and scanning electron microscopy (SEM), and the electrochemical behaviour was studied through three-electrode cell experiments. To assess the real applicability, their performance was contrasted to those of commercial carbon felts and non-woven fabrics. Enhanced vanadium REDOX activity in comparison to commercial options were observed, which proves the potential of these sustainable and novel materials as electrodes with enhanced electrocatalytic activity in different energy storage devices.

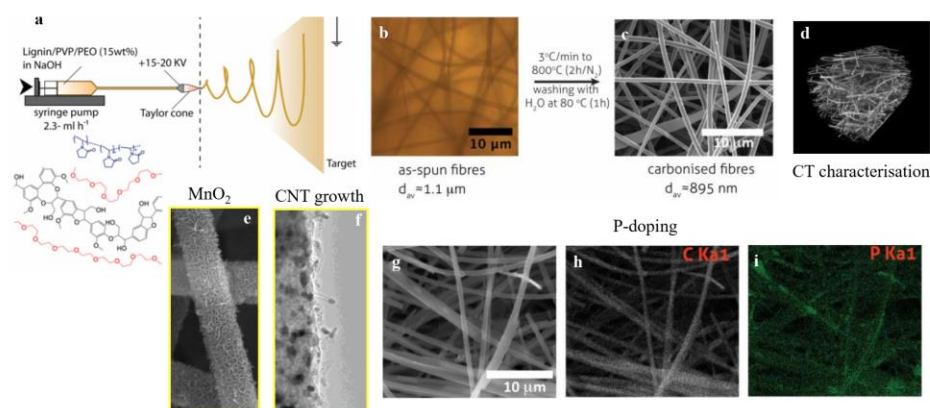


Figure 1. a) Scheme of lignin electrospinning, b) As-spun lignin fibres, c) Carbonised lignin fibres, d) CT imaging of carbonised lignin fibres, e) MnO₂-decorated carbon fibres, f) CNT-growth on carbon fibres; g), h) and i) Phosphorous doped carbon fibres.



Printed functional nanomaterials for optoelectronic applications

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More than 20% of the world's total electricity consumption is used for lighting applications. This number reaches 25% when consumption from display and TV applications is included. Therefore innovative, cost and energy effective solutions for display and lighting applications are the focus of an on-going intense world-wide effort in the field of photonics research and development activities. In particular, organic light-emitting diodes (OLEDs), alongside with inorganic solid-state lighting technologies, are the most promising candidates for future display and lighting technologies of the 21st century. The realization of lightweight, potentially flexible and cheap-to-fabricate, highly energy efficient lighting and display applications may help to save hundreds of GWh or millions tons of coal per year.

While the first report on organic electroluminescence from an organic semiconductor – an anthracene crystal - dates back to the 1960s, the discovery of thin film organic light-emitting device from Eastman Kodak by Ching W. Tang and Steven Van Slyke, and three years later, a report of the first polymer light-emitting diode (PLED) by R. Friend and associates triggered enormous efforts, both within academic research as well as industrial development. Yet, despite this first promising commercial success of OLED technologies, a number of challenges need to be further addressed to allow full exploitation of its potential. Along with the ever on-going quest for emitter materials with improved stability and reliable structure to property relations and enhanced processability through printing techniques in particular device related issues will be discussed in this contribution. In particular we report on the design, realisation and characterization of novel low temperature processes for printed electrode materials on flexible low cost substrates.



Implementing hydrothermal synthesis for novel fluorescent cell-staining dyes

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Fluorescence imaging is a widely employed technique in molecular biology to visualize biological events with a high spatial and temporal accuracy.¹ Among the existent fluorescent probes, small organic fluorescent dyes occupy a prominent position as they are (i) significantly easier to use than other techniques, (ii) and their properties relevant to cell staining applications (e.g. quantum yield, wavelength of emission, and solubility) can be modulated by chemical design.² The vast majority of fluorescent dyes currently used for cell staining are based on a small set of molecular scaffolds such as coumarins, fluoresceins, or rhodamines, and advances in the field of cellular stains are to date confined to the structural modification of the latter. Hence, the field heavily lacks structural diversity of stains. Synthetically, the preparation of cell stains requires – depending on the complexity of the scaffold – classical organic synthesis involving multistep reactions and tedious purification. Clearly, more efficient routes are highly desirable and hydrothermal synthesis (HTS) has been shown to be a novel and more environmentally friendly alternative to synthesize organic heterocycle- and aromatics-bearing compounds with high yields and shorter reaction times.³ In this talk, the synthesis of novel fluorescent dyes employing HTS as a key reaction step will be presented. The fluorescence properties both in the solid state and in solution of the dyes will be presented. Our results showcase that HTS can indeed be implemented in the synthesis of rather complex small organic molecules.

Supported by the Vienna Science and Technology Fund (WWTF) under the Grant “3C- Cellular Color Chart” (LS17-051)

¹ K. Thorn, *Mol. Biol. Cell.* **2016**, 27, 219. DOI: 10.1091/mbc.E15-02-0088

² Lavis, L. et. al, *ACS Chem. Biol.* **2014**, 9, 855. DOI: 10.1021/cb500078u

³ B. Baumgartner. et al, *Chem. Commun.* **2017**, 53, 1229. DOI: 10.1039/C6CC06567H



Triplet-triplet annihilation photon upconversion via macromolecular annihilators

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Use of solar energy is an attractive topic in materials science for nearly fifty years since traditional energy sources are limited, expensive, and have serious waste management problems.^[1,2] One of the major challenges faced during valorisation of photosystems is collecting the solar radiation in the specific region required by the corresponding process.^[3,4] In that context, triplet-triplet annihilation (TTA) photon upconversion (UC) is a useful method to improve the performance of the key material (i.e. the catalyst in photocatalysis, active layer of the solar cells) via converting the low energy segments to produce useful radiation for the desired application.^[5,6]

The TTA-UC process basically takes place between a sensitizer and an annihilator, which the former should be absorbing light in the lower energy area of the spectrum in order to produce triplet level excited electrons while the latter should have adequate energy levels to receive those electrons to upconvert them in order to emit light in higher energies than the initially absorbed one (Figure 1).^[6]

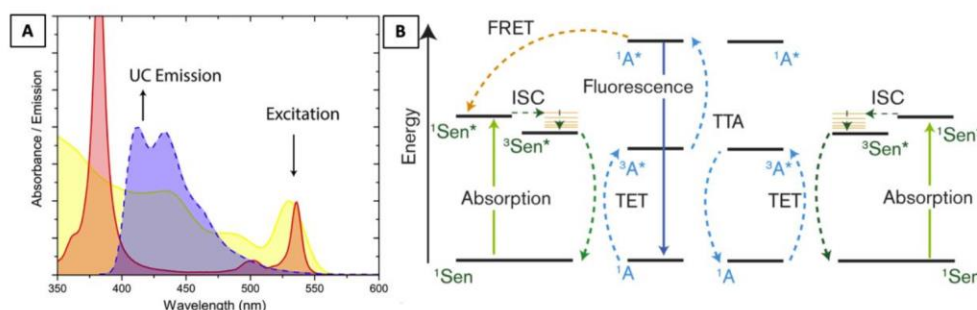


Figure 1 A) Excitation of the sensitizer in long wavelength and produced emission by annihilator in shorter wavelengths and B) mechanism of TTA-UC via Jablonski energy diagram (from ref 6).

The presentation will focus on novel approaches to yield better efficiencies in TTA-UC process by using anthracene based macromolecular annihilators. The advantages and challenges of such macromolecular systems will be discussed while comparing their performances with the benchmark material, namely 9,10-diphenylanthracene.

- [1] A. Louwen, et al., *Nat. Commun.* **2016**, 7, 13728. [2] N. S. Lewis, *Science* **2016**, 351, 1920. [3] K. T. Fountaine, et al., *Nat. Commun.* **2016**, 7, 13706. [4] J. H. Montoya, et al., *Nat. Mater.* **2016**, 16, 70. [5] B. D. Ravetz, et al., *Nature* **2019**, 565, 343. [6] V. Gray, et al., *Coord. Chem. Rev.* **2018**, 362, 54.



Catalytic inverse vulcanisation

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The discovery of ‘inverse vulcanisation’ has allowed stable polymers to be made from elemental sulfur, an unwanted by-product of the petrochemicals industry. However, further development of both the chemistry and applications is handicapped by the restricted choice of cross-linkers and the elevated temperatures required for polymerisation. We report the first catalysis of inverse vulcanization reactions.¹ This catalytic method was tested for a wide range of crosslinkers and found to reduce the required reaction temperature and reaction time, prevent harmful H₂S production, increase yield, improve properties, and allow crosslinkers that would be otherwise unreactive to be used. Thus, inverse vulcanization becomes more widely applicable, efficient, eco-friendly and productive than the previous routes, not only broadening the fundamental chemistry itself, but also opening the door for the industrialization and broad application of these fascinating new materials.

Supported by a Royal Society University Research Fellowship.



Figure 1. A range of moulded sulfur-polymers made using catalytic inverse vulcanisation, each from 50 wt.% sulfur, and each reacted with a different crosslinker. Elemental sulfur powder and an example of an organic crosslinker shown at rear of image.

¹ X. Wu et al., *Nature Communications*, **2019**, 10, 647. DOI: 10.1038/s41467-019-08430-8



Synthesis of nitrogen doped porous carbon microspheres using metal assisted polymerization strategy for efficient oxygen reduction reaction

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Oxygen reduction is a reaction of prime interest that is playing central roles in metal-air batteries and fuel cells. Currently, expensive metals like Pt, Ru and Ir are being used for the catalysis of oxygen reduction reaction (ORR) in alkaline or acidic media. The ORR efficiency is affected by poor mass transport, high overpotentials, poor durability, CO and methanol poisoning. It is thus increasingly important to prepare inexpensive, nonprecious, porous carboneaceous catalysts using a strategy that is simple, sustainable, and cost-effective.

Herein, a metal assisted polymerization strategy to preparing nonprecious nitrogen doped porous carboneaceous catalysts is presented. The polymerization of a conducting polymer like pyrrole is initiated by metal caps collected from waste Zn-C battery under acidic conditions at room temperature to form polypyrrole microspheres, which are then activated and carbonized under inert atmosphere to form nitrogen doped porous carbon microspheres (Fig. 1). The porosity and the surface area of the nitrogen doped porous carbon microspheres is controlled by changing the carbon to activating agent mass ratios and the activation time. The as-prepared nitrogen doped porous carbon spheres showed improved ORR activity under alkaline medium and the activity is several fold higher than that of smooth carbon spheres. With the advantages of low-cost preparation, porosity and nitrogen doping, as-prepared nitrogen doped porous carbon microspheres are holding great potential use in alkaline fuel cells.

Supported by the following Grant (SEMA1M1R).

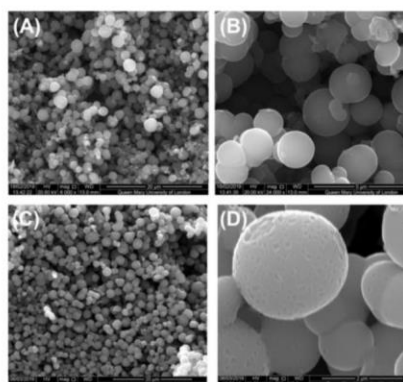


Figure 1. SEM images of nitrogen doped smooth carbon spheres (A, B) and nitrogen doped porous carbon spheres (C, D).



Cobalt-exchanged poly(heptazine imides) as transition metal-N_x electrocatalysts for oxygen evolution reaction

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Metal-N_x sites are well-known as highly-active catalytic sites in electrocatalysis for various electrocatalytic reactions.^{1,2} Poly(heptazine imide) is a new family member of polymeric carbon nitride. Due to its defined structure, good conductivity and abundant and well-dispersed negatively charged nitrogen sites, poly(heptazine imide) is a promising material for designing Metal-N_x electrocatalysts.³ In this work, poly(heptazine imide)s hosting cobalt ions as counteranions are presented as promising electrocatalysts for the oxygen evolution reaction (OER). A facile mixed salt-melt assisted condensation was developed to prepare such cobalt poly(heptazine imide)s (PHI-Co). The Co ions can be introduced in well-controllable amounts using this method and are shown to be atomically dispersed within the imide-linked heptazine matrix. When applied to electrocatalytic OER, PHI-Co's showed a remarkable activity with an overpotential of 324 mV and Tafel slope of 43 mV/dec in 1M KOH.

This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – EXC 2008/1 (UniSysCat)– 390540038.

¹ Wu, G.; Santandreu, A.; Kellogg, W.; Gupta, S.; Ogoke, O.; Zhang, H.; Wang, H. L.; Dai, L. *Nano Energy*, 29, 83–110(2016).

² Tang, Y.; Liu, R.; Liu, S.; Zheng, B.; Lu, Y.; Fu, R.; Wu, D.; Zhang, M.; Rong, M. *Carbon N. Y.*, 141, 704–711(2019).

³ Chen, Z.; Savateev, A.; Pronkin, S.; Papaefthimiou, V.; Wolff, C.; Willinger, M. G.; Willinger, E.; Neher, D.; Antonietti, M.; Dontsova, D. *Adv. Mater.* 29 (32), 1–8 (2017)



Nanosized niobium pentoxide acid catalysts with varying acidity: Insights into the structure-acidity-activity relationships of Nb₂O₅

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Niobium pentoxides (e.g. amorphous Nb₂O₅·*n*H₂O) are promising acid catalysts for the conversion of biomass to valuable chemicals in biorefineries. However, the development of Nb₂O₅ catalysts for specific practical processes is hindered by the limited number of synthesis routes available to achieve structural modifications and consequent incomplete understanding of their structure-acidity-activity relationships. Here, we present a synthesis route in acetophenone to highly hydroxylated nano-structured Nb₂O₅ with varying structural motifs and acidity that efficiently catalyze the etherification and esterification reactions of furfuryl alcohol, 5-(hydroxymethyl)furfural and α-angelica lactone. The oxides have orthorhombic structures with different extents of distortions and coordinatively unsaturated metal atoms. A strong dependence is observed between the type and strength of the acid sites and specific structural motifs in the solids. A structure based mainly on corner-shared octahedra, as that of orthorhombic Nb₂O₅, leads to medium-weak Brønsted acid sites. Strong Brønsted acidity is generated by distortions in the orthorhombic structure, associated with protonated oxygen atoms. Lewis acid sites originate from highly distorted structural units that tend to form in structures with higher degrees of disorder.

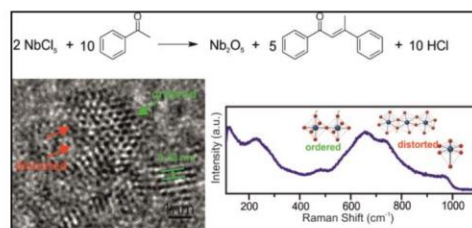


Figure 1: Niobium pentoxides synthesis and structural characterization.

Supported by the DFG, Grant no. RU2012/2-1



Water-equilibrated high-O₂-soluble ionic liquids make nanocarbon more active and stable for oxygen reduction catalysis

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Clean electricity can be generated in a Proton Electrolyte Membrane Fuel Cell (PEMFC) when diatomic hydrogen molecules are split into hydrogen ions and free electrons at the anode, by passing the generated proton through the electrolyte over a catalyst at the cathode to react with oxygen and produce water as the only by-product. So far, the 'practical' catalysts known for the so-called Oxygen Reduction Reaction (ORR) at the cathode of PEMFC are platinum-group metals primarily metallic platinum (Pt). Therefore, the use of scarce metals is a huge problem hindering the commercialization of fuel cells.

Here we want to present an innovative and revolutionary concept used to improve even further PEMFC's performance without using Pt catalysts. This new concept is based on the addition of an ionic liquid which is oxygenophilic (promotes oxygen adsorption onto the catalytic active site) and hydrophobic (repels water preventing the formation of hydrogen peroxide) to our Pt-free electrocatalyst during the electrode preparation. We have demonstrated this concept for two ionic liquids, protic ionic liquid 1-Ethylimidazolium bis (trifluoromethylsulfonyl) imide ([C₂im][NTf₂]), and aprotic ionic liquids 1-butyl-3-methylimidazolium bis (trifluoromethanesulfonyl) imide ([C₄C₁im][NTf₂]) was chosen to modify the catalyst-electrolyte interfacial microenvironment. The ionic liquid layers at nanocarbon surface provide a water-equilibrated secondary medium with a higher O₂ solubility, meanwhile hydrophobic nature preventing water build-up locally, and also provide sufficient H⁺/H₃O⁺/OH⁻ conductivity. This modification strategy exhibits a remarkable improvement for ORR in both alkaline and acid electrolyte in regarding to the catalytic activity and long-term stability. This work offers a new direction for the optimization of nanocarbon-based electrocatalysts, and provide some fresh insights in the design principles. It possesses the potential to be further developed into a universal technique to successfully ameliorate the surface property of advanced nanocarbon materials, aiming at applications in various fields, such as Li-ion batteries, supercapacitors, sensors, etc.



Inverse vulcanised sulfur polymers for functional materials

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Inverse vulcanised sulfur polymers are exciting, promising, novel materials that provide an excellent alternative to carbon based polymers. More than 60 million tonnes of excess sulfur is produced annually by hydrodesulfurisation of crude oil and gas (Fig 1a).¹ Recent research into inverse vulcanisation has shown how this excess sulfur can be transformed into functional polymers, by stabilisation with organic crosslinkers (Fig 1b).¹ Here we discuss our findings on how innovative inverse vulcanised sulfur polymers can be utilised for very different applications.

We discuss how different sulfur polymers can be used to remove mercury from water, in particular the removal of 2-methoxyethylmercury chloride (MEMC), an organofungicide still used today on sugar cane crops in Australia (Fig 1c). This compound is not only detrimental to human health of farmers and those nearby, but also flags major concerns for aquatic life. Alongside this, we show how we can control polymeric properties by preparing novel terpolymers prepared from sulfur and two different alkene monomers, tuning glass transition, molecular weight, solubility, mechanical properties and colour (Fig 1d). We also report a new system using 5-Ethylidene-2norbornene as a crosslinker which can stabilise up to 90 wt. % of elemental sulfur and combine synthesis, spectroscopy and modelling to reveal structure-property relationships (Fig 1e).² Finally, new findings on the antimicrobial properties of these novel polymeric materials will be discussed, reporting a bacterial log₁₀ reduction of >4 on exposure to *Staphylococcus aureus*.

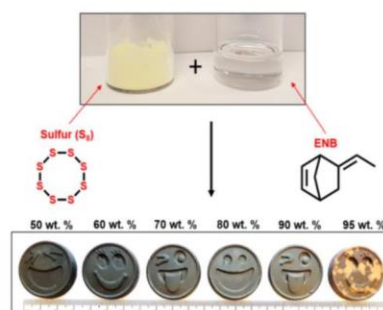


Figure 1. Top: elemental sulfur (left) and ENB crosslinker (right). Bottom: S-ENB polymers 50, 60, 70, 80, 90 and 95 wt% elemental sulfur.

¹Pyun *et al*, *Nature Chemistry*, **2013**, 5, 518-524. DOI: 10.1038/nchem.1624

²J.A.Smith *et al.*, *Journal of Polymer Science Part A*, **2018**, 56, 1777-1781. DOI: 10.1002/pola.29067



Hard-soft carbon composite anodes with synergistic sodium storage performance

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Carbonaceous materials, especially hard carbons, are regarded as the most promising candidates as anode materials for SIBs among other choices such as titanium-based materials, chalcogen-based materials, alloys and organic materials, owing to advantages such as performance, cost, sustainability and structural stability.¹ But pure hard carbons usually show very low capacity and initial Coulombic efficiency due to their high specific surface area when carbonized at low temperatures (below 1000 °C). Therefore, hard carbon anodes are normally treated at temperatures above 1300 °C, which adds extra costs, in addition to that from the precursor. Here we present the production of hard-soft composite with higher capacity and initial Coulombic efficiency at a low carbonization temperature of 1000 °C compared to pure hard or soft carbon treated at the same temperature. This synergy is achieved by blocking the open pores and decreasing the surface area and Na⁺ ions consumption during solid electrolyte interface (SEI) formation, while maintaining a large number of sodium storage sites.

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¹ Q. Wang et. al, *Small* **2017**, 1701835 DOI: 10.1002/sml.201701835



Vanillin-based polymer as a sustainable alternative for cathodes in lithium-ion batteries

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Batteries are everywhere around us and are soon to replace the fuel tank of our cars. Therefore there is a growing demand for cheaper batteries from renewable resources. Lignin is a naturally occurring polymer found in wood and a low value side product in many industries such as paper industry. Previously, usage of lignin as a cathode material in secondary batteries has been reported, employing hydroquinone analogues in lignin's structure that undergo reversible electrochemical transformation to quinone analogues.¹ However, due to the complicated structure of lignin, cathodes for lithium ion batteries were not prepared successfully.

Instead using lignin as such for energy storage, it can be used as a feedstock to produce low molecular weight molecules containing the same active groups as lignin but at a higher density. One of the most prominent lignin based small molecules is vanillin. Because of tremendous demand, efficient and economical routes have been developed to industrially synthesize it from lignin. After easy functionalization using only sustainable solvents such as acetic acid and water, we now synthesized a sustainable polymer with a high density of electrochemically active functional groups. Special focus has been given to a new method of polymerization in the presence of a porous carbon material, leading to the formation of a functional hybrid material and allowing for the omission of binder. Resulting electrodes are stable, porous, conductive, redox-active, and – most importantly – derived from renewable resources and thus may be used in future green energy storage devices.

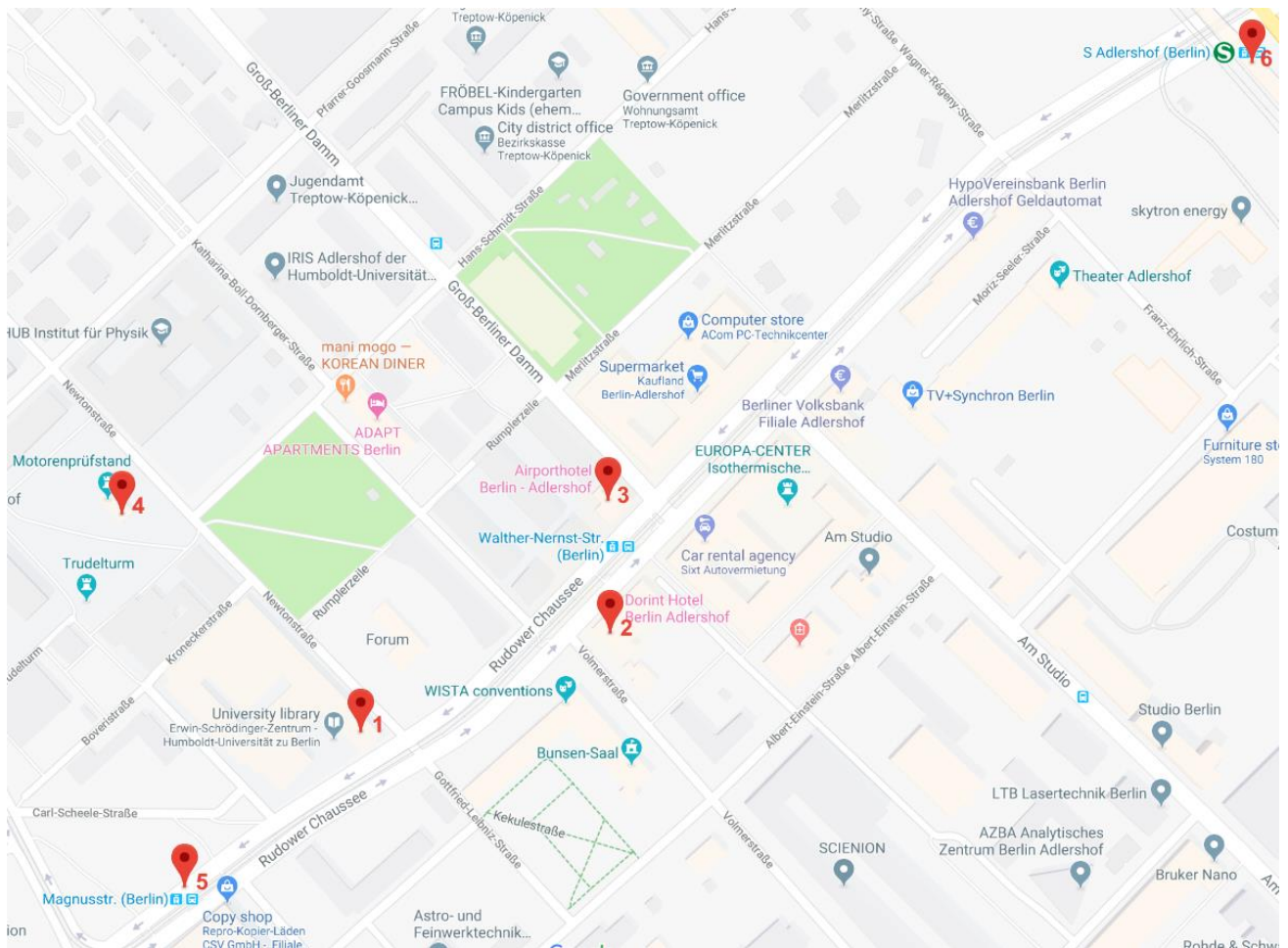
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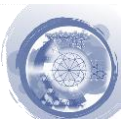
¹ O. Milczarek, Grzegorz; Inganas, *Science* (80-.). **2012**, 335, 1468–1471



POINTS OF INTEREST

1. **Erwin-Schrödinger-Zentrum**, Rudower Chaussee 26, 12489 Berlin
2. Dorint Hotel Berlin Adlershof <https://hotel-berlin-adlershof.dorint.com/en/>
3. Airporthotel Berlin-Adlershof <http://www.airporthotel-berlin-adlershof.de/?lang=en>
4. Student bar “Motorenprüfstand”
5. Nearest tram station (Tram 61, 63) “Magnusstr.”
6. Nearest commuter train station (S Bahn S8, S9, S45, S46, S85) “Adlershof”

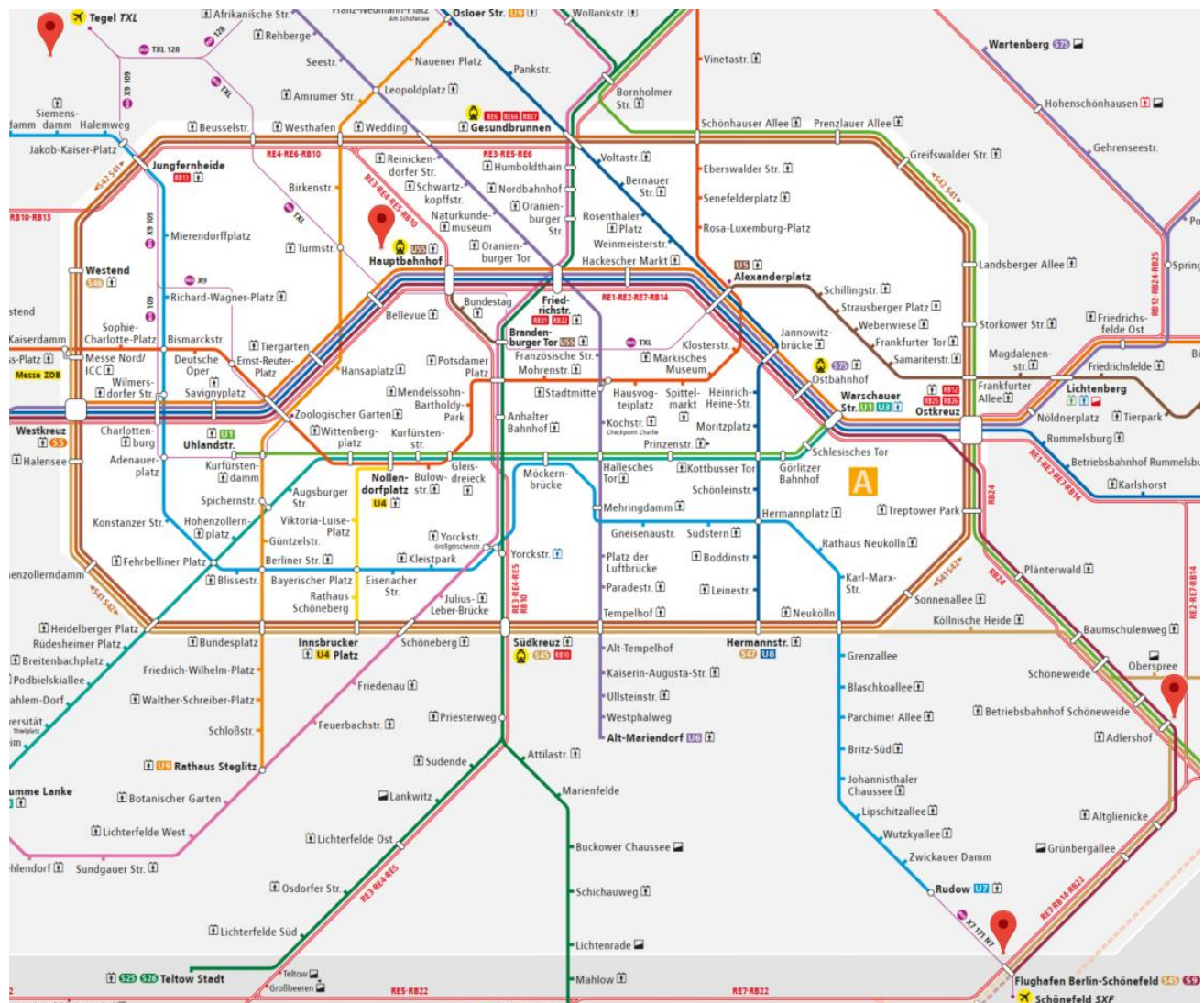


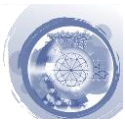


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