KOPO 2024

CONJUGATED OLIGOMERS AND POLYMERS

From Molecules to Materials

12th Workshop
May 26-29, 2024
Physikzentrum Bad Honnef

UNIVERSITÄT BONN

Location

Physikzentrum Bad Honnef
Hauptstr. 5
53604 Bad Honnef
http://www.dpg-physik.de/dpg/pbh

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Contents

Sunday, May 26, 2024

15:30 – 17:00	*Registration & Coffee reception*
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17:15 – 18:00	*Rudolph-Gompper-Memorial Lecture:* **Frank Würthner:** Supramolecular Engineering of Functional Materials
18:00 – 18:30	*Time to prepare poster session*
18:30 – 20: 30	*Dinner*
20:30	*Workshop Mixer*

Monday, May 27, 2024

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Chair: Arne Lützen

09:00 – 10:00	*Plenary lecture* **Birgit Esser:** Organic Materials: From Batteries to Conjugated Nanohoops
10:00 – 10:25	**Liping Ye:** Synthesis of Electronic Delocalized Möbius Belt
10:25 – 10:50	**Eric Sidler:** Redox-Switchable Aromaticity in a Helically Extended Indeno[2,1 c]fluorene
10:50 – 11:10	*Coffee Break*

Chair: Birgit Esser

11:10 – 11:35	**Klaus Meerholz:** Non-Fullerene Acceptors in Organic Solar Cells – Some new Insights
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12:00 – 12:25	**Luisa Rieger:** Molecular conductance of diaryl amine capped carbon-bridged oligo(phenylene vinylene)s
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Chair: Klaus Meerholz

14:00 – 14:25	**Princekumar Ravat**: Molecular Engineering of Helically Chiral Functional Molecules: Materials for Next Generation (Opto)electronics
14:25 – 14:50	**Rajeev Dubey:** Charge-transfer supported supramolecular host–guest interactions in a tailored hexabenzocoronene host
14:50 – 15:15	**Philipp Krämer:** A Lateral Expansion Strategy for all-phenylene Molecular Spoked Wheels
15:15 – 16:00	*Coffee Break*

Chair: Princekumar Ravat

16:00 – 16:25	**Hans-Achim Wagenknecht:** Supramolecular DNA Architectures with Chromophores
16:25 – 16:50	**Felix Majer:** Through-space charge transfer in anthracene-based emitters – a new paradigm for TADF molecules
16:50 – 17:10	**Jake Greenfield:** Switching It Up: Enhancing the Photochromic Behavior of Imines
18:00 – 19:30	*Dinner*
19:30	**Poster Session**

Tuesday, May 28, 2024

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09:00 –10:00	*Plenary lecture* **Xinliang Feng:** Two-Dimensional Conjugated Polymers: From Dream to Reality
10:00 – 10:25	**Sven Elbert:** A Negatively Curved Nanographene with four embedded Seven-membered Rings and its Supramolecular Interactions with Fullerenes
10:25 – 10:50	**Giulia Lavarda:** Supramolecular polymers as model systems for organic optoelectronics
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Chair: Xinliang Feng

11:10 – 11:35	**Erik Misselwitz**: Indenoannulated Tridecacyclene: An All-Carbon Seven-Stage Redox-Amphoter
11:35 – 12:00	**Moritz Nau:** Conformationally Regulated Molecular Conductance Switching in Arylene-Bridged Bis(Triarylamines**)**
12:00 – 12:25	**Leon Euringer:** Tuning Electron Transfer Coupling and Exchange Interaction in Bis triarylamine Radical Cations and Dications by Bridge Electron Density

13:00 – 14:00	*Lunch*
14:30	Excursion: Visit to the Arithmeum, dinner at the Rheinlust restaurant (bus tour)

Wednesday, May 29, 2024

07:30 – 09:00 *Breakfast*

Chair: Milan Kivala

09:00 – 10:00 *Plenary lecture*
Colin Nuckolls: Creating Functional Materials from Contorted Aromatic Building Blocks

10:00 – 10:25 **Robert Eichelmann:** Tetraazacoronenes

10:25 – 10:50 **Wenhui Niu:** Multilayer Helical Nanographenes with Layer-Dependent Chiroptical Properties

10:50 – 11:10 *Coffee Break*

Chair Sigurd Höger

11:10 – 11:35 **Christoph Keck:** Synthesis of Chiral Pyrene-Based 1,4-Dithiins

11:35 – 12:00 **Charlotte Kress**: Outstanding Chiroptical Properties of Conjugated Polygon-Shaped Macrocycles

12:00 – 12:25 **Jan Borstelmann:** Helically Chiral π-Expanded Azocines Through Regioselective Beckmann Rearrangement and Their Charged States

12:25 – 12:50 **Marvin Schumacher:** Added Value of Circular Dichroism for Studying Charge Transfer Excitons in Photoactive Organic Thin Films

12:50 **Closing Remarks:** Arne Lützen, Sigurd Höger

13:00 *Lunch*

Rudolf Gompper Memorial Lecture

Supramolecular Engineering of Functional Materials

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For a period of more than twenty years our group has studied the formation of molecular aggregates and the functional properties originating from the interaction of various π-systems (merocyanines, squaraines, polycyclic aromatic imides) in terms of structure-function relationships. Dimers were of particular value because they can be synthesized easily and with their still modest size can be elucidated by higher level quantum chemical methods. In this lecture I will showcase perylene bisimides (PBIs), a class of materials characterized by a particularly rich functional complexity, originating from strong structure-dependent electronic couplings between the molecular building blocks. Thus, with a knowledge-based supramolecular engineering approach PBI-based molecular aggregates and materials can be engineered that exhibit desirable properties for a variety of applications from traditional colorants up to solid state emission and organic electronics.

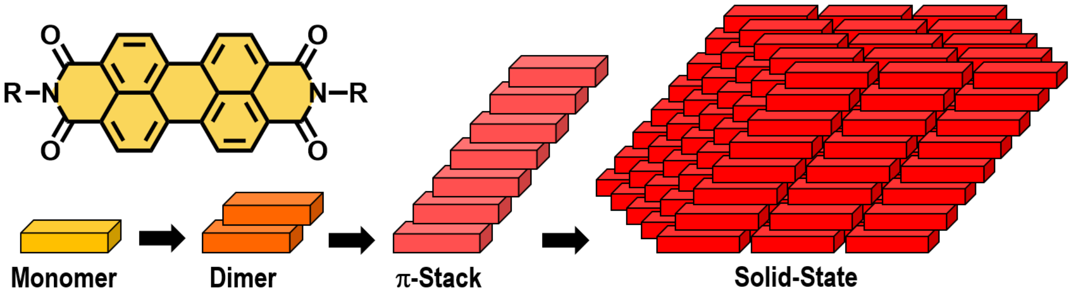

Figure 1: Molecular matter from monomers via aggregates up to solid state materials.

References:

[1] R. K. Dubey, F. Würthner, *Nat. Chem.* **2023**, *15*, 884: Playing Lego with perylene dyes
[2] F. Würthner, C. R. Saha-Möller, B. Fimmel, S. Ogi, P. Leowanawat, D. Schmidt, *Chem. Rev.* **2016**, *116*, 962–1052: Perylene Bisimide Dye Assemblies as Archetype Functional Supramolecular Materials

Plenary Lectures

Organic Materials: From Batteries to Conjugated Nanohoops

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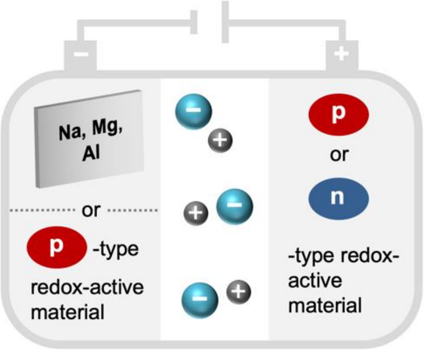
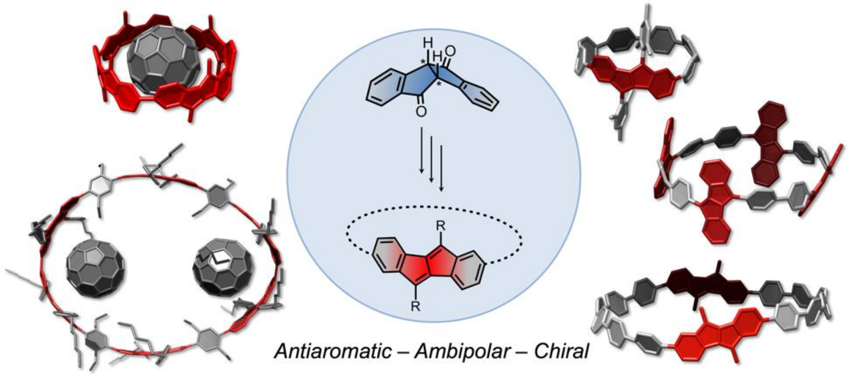
In face of the climate change there is a strong and growing demand for the storage of renewable energies. Organic electrode materials have attracted great interest for next-generation batteries, as they can be prepared from renewable, sustainable or less-limited resources, they are easy to recycle as well as potentially safer and cheaper to produce. Both p- and n-type organic materials with reversible redox processes can be used, often based on π-systems, furnishing different types of cell configurations.[1] In the first part of this talk design principles and examples of organic battery electrode materials and their application in all-organic and multivalent metal full cells will be discussed.



In conjugated nanohoops the effect of radial conjugation and bending on the π-systems can be investigated, they can possess unexpected optoelectronic properties, and their radially oriented π-system makes them attractive for host-guest chemistry. With the right choice of a π-subsystem, bending it out of planarity can induce chirality in the hoop. Dibenzopentalene is a small-bandgap, ambipolar organic semiconductor, which also makes it attractive for organic field-effect transistors. In the second part of this talk, synthetic strategies to (enantiopure) dibenzopentalene-based nanohoops will be presented as well as their optoelectronic, host-guest and chiroptical properties discussed.[2]



References:

[1] (a) B. Esser, F. Dolhem, M. Becuwe, P. Poizot, A. Vlad, D. Brandell, *J. Power Sources* **2021**, *482*, 228814; (b) B. Esser, *Org. Mater.* **2019**, *01*, 063–070.

[2] B. Esser, J. S Wössner, M. Hermann, *Synlett* **2022**, *33*, 737–753.

Two-Dimensional Conjugated Polymers: From Dream to Reality

Xinliang Feng

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Two-dimensional (2D) conjugated polymers have been a highly sought-after class of polymeric materials in the synthetic polymer and organic electronics communities. The extensive conjugation in two dimensions can, in principle, offer the possibility to confront the major challenges faced by linear polymer semiconductors. The sheet-like network can be regarded as n-strand ladder chains, where charge carriers can travel through the different chains, and therefore, bypass the possible defects and grain boundaries with the hopping mechanism that is commonly present in linear conjugated polymers. The unique structural features and electronic band structures would render 2D conjugated polymers highly promising candidates for next-generation electronic, optoelectronic, and spintronic devices.

However, synthetic chemistry methodologies to achieve extensive 2D conjugation and efficient 2D polymerization have yet to be developed. Classical dynamic covalent chemistry commonly used in covalent organic frameworks, and topochemical polymerization strategies, fail to provide 2D conjugated polymers with required structural features, let alone access to their unique properties. In this lecture, we will present our recent efforts towards the design and synthesis of crystalline 2D conjugated polymers. In the first part, we will focus on solution-based 2D polymerization, including the Knoevenagel reaction, HWE reaction, and Wittig reaction, to synthesize 2D polyarylenevinylenes (2D PAVs) in a robust manner. The C=C conjugation linkage provides excellent conjugation pathways for 2D PAVs, as evidenced by the decreased optoelectronic bandgaps, and reasonable charge carrier transport properties through the studies using THz spectroscopy methods, etc. Additionally, we will demonstrate the development of 2D PAVs for high-performance photoelectrochemical water splitting. In the second part, theoretical design is utilized to guide the synthesis of 2D conjugated polymers with extensive conjugation. We will demonstrate the synthesis of 2D benzimidazobenzophenanthroline (BBL)-type ladder-type conjugated polymers, which exhibit enhanced band-dispersion and outstanding charge carrier mobilities (~1000 $cm^2V^{-1}s^{-1}$ at room temperature). In the final part, we will discuss the on-water surface chemistry to synthesize 2D conjugated polymer crystals, ranging from monolayer to a few layers. In particular, we will highlight the synthesis of unprecedented 2D polyaniline crystals. The unique anisotropic metallic state of 2D polyaniline crystals will also be demonstrated.

Wang, M. et al. *Nat. Mater.* **2023**, *22*, 880; Liu, Y. et al. *Angew. Chem. Int. Ed.* **2023**, e202305978; Liu, Y. et al. *Angew. Chem. Int. Ed.* **2022**, e202209762; Xu, S. et al. *Angew. Chem. Int. Ed.* **2022**, *61*, e202202492; Wang, Z. et al. *Nat. Synth.* **2022***, 1,* 69; Xu, S. et al. *Adv. Mater.* **2021**, *33,* 2006274; Xu, S. et al. *Acc. Mater. Res.* **2021**, *2*, *4*, 252; Liu, K. et al. *Angew. Chem. Int. Ed.* **2021**, *60,* 1-7; Seki, T. et al. *Chem* **2021***, 7*, 2758; Pastoetter, D. et al. *Angew. Chem. Int. Ed.* **2020**, *59*, 23620; Wang, M. et al. *J. Am. Chem. Soc.* **2020**, *142*, 52, 21622; Wang, M. et al. *J. Am. Chem. Soc.* **2019**, *141*, 42, 16810; Xu, S. et al. *Angew. Chem. Int. Ed.* **2019**, *58*, 849; Zhang, T. et al. *Nat. Commun.* **2019**, *10*, 4225; Liu, K. et al. *Nat. Chem.* **2019**, *11*, 994; Dong, R. et al. *Nat. Mater.* **2018**, *17*, 1027; Zhuang, X. et al. *Polym. Chem.* **2016**, *7*, 4176; Sahabudeen, H. et al. *Nat. Commun.* **2016,** *7*, 13461.

Creating Functional Materials from Contorted Aromatic Building Blocks

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This presentation will detail our efforts to create materials from contorted aromatic molecules. In particular, I will discuss how to create ladder polymers from helicenes and twistacenes building blocks. These materials have extraordinary properties as materials. The helicenes have the largest chiroptic response of any molecular species. The twistacenes excel as photovoltaics, photodetectors, batteries, and pseudocapacitors. The presentation will discuss these opportunities.

Lectures

Helically Chiral π-Expanded Azocines Through Regioselective Beckmann Rearrangement and Their Charged States

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We report a synthetic approach to π-expanded [6]helicenes incorporating tropone and azocine units in combination with a 5-membered ring, which exhibit intriguing structural, electronic, and chiroptical properties. A regioselective Beckmann rearrangement allows the isolation of helical scaffolds containing 8-membered lactame, azocine, and amine units, as confirmed by X-ray crystallography. The compounds exhibit notable optoelectronic properties depending on the relative position of the nitrogen. Chiral resolution of all helical compounds allows comprehensive investigation of the chiroptical properties by CD and CPL measurements. The azocine compounds feature rich redox chemistry allowing for characterization of the respective monocations and monoanions, as well as dications and dianions with NIR absorption beyond 3000 nm (Figure 1).[1]

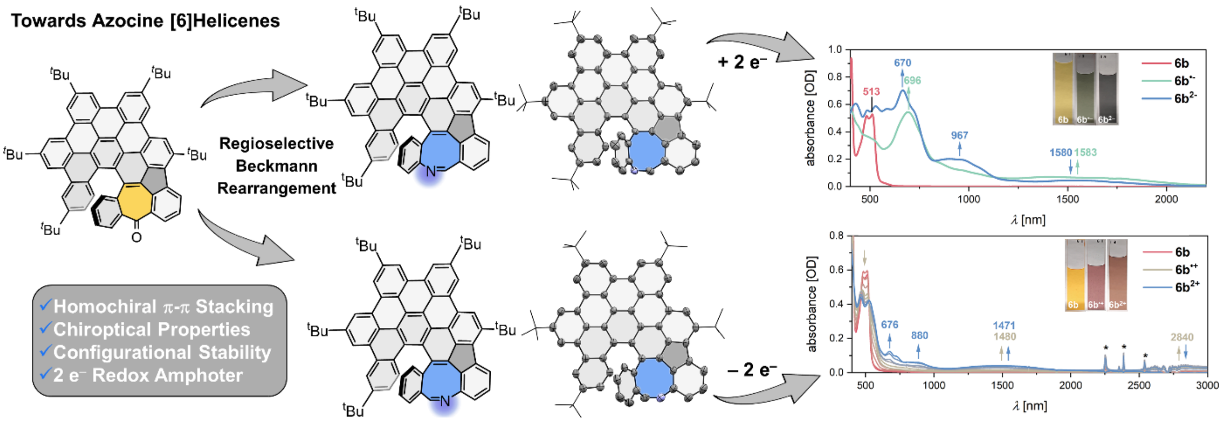

Figure 1: Regioselective Beckmann rearrangement leads to helical azocines with distinct optoelectronic properties and interesting redox chemistry.

References:

[1] J. Borstelmann, L. Schneider, F. Rominger, F. Deschler, M. Kivala, *manuscript submitted*.

Poly(arylene iminoboranes): A new Class of Inorganic–Organic Hybrid Polymers with a B=N Doped Backbone

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The substitution of selected CC units by isoelectronic and isosteric BN units in polyaromatic compounds has evolved into a powerful approach for accessing novel materials with modified, often intriguing properties and functions.[1] We reported the first poly(*p*-phenylene iminoborane), which is derived from PPV through replacement of its vinylene by B=N moieties (i.e., BN-PPV).[2] Next, we targeted a BN/CC isostere of poly(thiophene vinylene) (PTV), namely, a poly(thiophene iminoborane) (BN-PTV),[3] as well as mixed copolymer congeners of both PPV and PTV.[4] The polymers and a series of monodisperse oligomers showed solid-state fluorescence and pronounced π-conjugation over the B=N units. We recently also accomplished the synthesis of a regioregular BN-PPV (*rr*-BN-PPV) and corresponding monodisperse oligomers, which showed fluorescence emission from a twisted intramolecular charge transfer (TICT) state.

Figure 1: Structures of BN-PPV, BN-PTV and their films under UV light, as well as *rr*-BN-PPV.

References:

[1] a) M. J. D. Bosdet, W. E. Piers, *Can. J. Chem.* **2009**, *87*, 8-29; b) H. Helten, *Chem. Eur. J.* **2016**, *22*, 12972-12982; c) Z. X. Giustra, S.-Y. Liu, *J. Am. Chem. Soc.* **2018**, *140*, 1184-1194.
[2] T. Lorenz, M. Crumbach, T. Eckert, A. Lik, H. Helten, *Angew. Chem. Int. Ed.* **2017**, *56*, 2780-2784.
[3] J. Chorbacher, M. Maier, J. Klopf, M. Fest, H. Helten, *Macromol. Rapid Commun.* **2023**, *44*, 2300278.
[4] M. Maier, J. Chorbacher, A. Hellinger, J. Klopf, J. Günther, H. Helten, *Chem. Eur. J.* **2023**, *29*, e202302767.

Charge-transfer supported supramolecular host–guest interactions in a tailored hexabenzocoronene host

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The vast majority of supramolecular host–guest systems based on π-conjugated molecules are governed by dispersion interactions between adjacent π-surfaces,[1] which most recently even allowed us to derive a correlation between the area of interacting π-surface and the Gibbs binding energy.[2] Herein, contrary to this common observation, we present our recent results from a detailed host–guest study on a hexabenzocoronene-based host (Figure 1) that illustrates the significance of charge-transfer interactions in supramolecular binding. In our study, polycyclic aromatic hydrocarbons (PAHs) showed poor binding and revealed no correlation between the size of the π-surface and the binding strength. However, electron deficient guests exhibited a substantial binding, and the binding strength was increased in relation to increased electron deficiency of the guest with the binding constant reaching up to 10^7 M^{-1} for the most electron deficient guest.

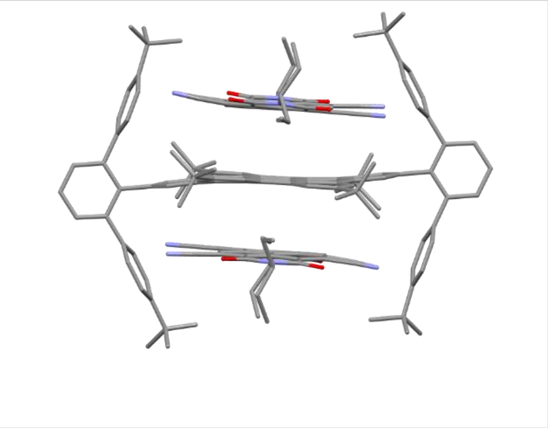

Figure 1: Hexabenzocoronene-based host with two encapsulated guests.

References:

[1] E. M. Perez, N. Martin, *Chem. Soc. Rev.* **2015**, *44*, 6425-6433.
[2] J. Rühe, M. Rajeevan, K. Shoyama, R. S. Swathi, F. Würthner, *Angew. Chem. Int. Ed.* **2024**, e202318451

Tetraazacoronenes

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The synthesis and characterization of *N*-substituted coronene derivatives and their laterally π-expanded congeners is presented. Recently, we have employed "*N*-doping" of PAHs as a means to modify their electronic properties while retaining their molecular shapes to the field of perylene chemistry.[1] Starting from a *bay*-chlorinated OAPPDO (**1**), tetraazacoronenes are accessible via fourfold Suzuki-Miyaura cross coupling or Zr-mediated cyclization.[2] Using bis(pinacolatoboryl)vinyl derivatives as ethylene building blocks,[2,3] the azacoronene parent compound and its corresponding condensed dimer, trimer and tetramer have been synthesized. All tetraazacoronenes display highly resolved UV/Vis absorption bands, pronounced fluorescence properties and an increased density of accessible redox states. This approach should allow the systematic investigation of this new class of functional dyes both in terms of their photophysics and their properties as molecular organic charge carriers.

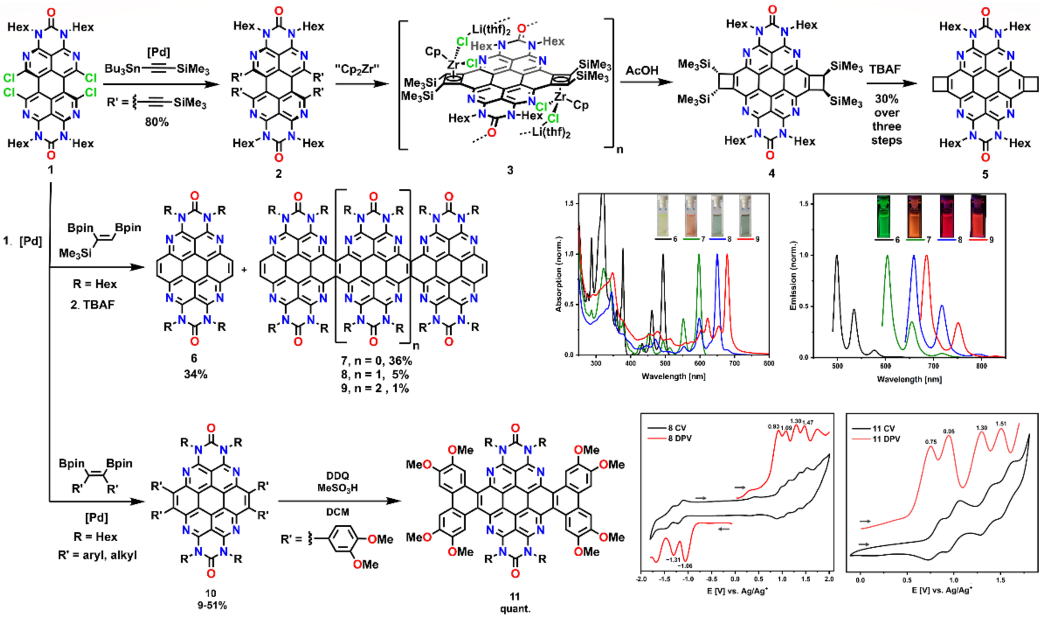

Figure 1: Synthesis and selected optoelectrical properties of tetraazacoronenes.

References:

[1] a) T. Wesp, T. Bruckhoff, J. Petry, H. Wadepohl, L. H. Gade, *Chem. Eur. J.* **2022**, *28*, e202200129; b) T. Wesp, P. Valsalan, A. Kochan, M. Hertzog, H. Wadepohl, J. Zaumseil, L. H. Gade, *Chem. Eur. J.* **2022**, *28*, e202202661; c) T. Wesp, T. Bruckhoff, H. Wadepohl, L. H. Gade, *Chem. Eur. J.* **2022**, *28*, e202201706.

[2] R. Eichelmann, J. Ballmann, L. H. Gade, *Angew. Chem. Int. Ed.* **2023**, *62*, e202309198.

[3] R. Eichelmann, D. Rippel, J. Ballmann, Lutz H. Gade, *Chem. Commun*. **2023**, *59*, 12136-12139.

A Negatively Curved Nanographene with four embedded Seven-membered Rings and its Supramolecular Interactions with Fullerenes

Sven M. Elbert, Owen T. A. Paine, Tobias Kirschbaum, Moritz P. Schuldt, Laura Weber,
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Fully sp^2-hybridised carbon allotropes are of fundamental scientific interest due to their unique physical properties as known for 0D (fullerenes), 1D (carbon nanotubes) or 2D (e.g. graphene) materials. However, approaches to conjugated 3D allotropes, such as Mackay-Terrones Schwarzite crystals (or short: Schwarzites),[1] are rare and limited in terms of structure elucidation as well as homogeneity.[2] Thus, there is a rising urge to synthesis discrete cut-outs of Schwarzites, namely negatively curved polycyclic aromatic hydrocarbons (PAHs). Although the introduction of eight and especially seven-membered rings is a common approach to create this class of PAHs, to the best of our knowledge there is only one example each for PAHs with four,[3] five[4] or six[3] seven-membered rings reported till date.

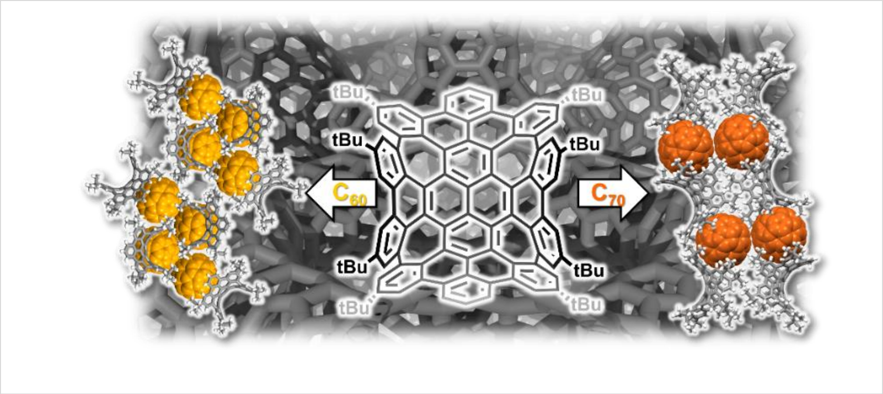

Figure 1: Schematically representation of a Negatively Curved Nanographene with four embedded Seven-membered Rings and cut-outs of single crystal X-ray structures with C_{60} (left) and C_{70} (right).

Here we present a saddle-shaped negatively curved PAH with four embedded seven-membered rings, that can be seen as a dibenzannulated cut-out of the Mackay crystal 6-1-1-p.[1] The negative curvature of the saddle was unambiguously proven by single crystal X-ray diffraction analysis (SCXRD) and due to the concave aromatic surface, supramolecular interactions with convex molecules such as the fullerenes C_{60} and C_{70} where studied in co-crystals by SCXRD as well as spectroscopic methods in solution.[5]

References:

[1] A. L. Mackay and H. Terrones, *Nature* **1991**, *352*, 762.
[2] a) Y. Segawa, H. Ito, K. Itami, *Nat. Rev. Mater.* **2016**, *1*, 15002; b) K. Kim, T. Lee, Y. Kwon, Y. Seo, J. Song, J. K. Park, H. Lee, J. Y. Park, H. Ihee, S. J. Cho, R. Ryoo, Nature **2016**, *535*, 131-135; c) E. Braun, Y. Lee, S. M. Moosavi, S. Barthel, R. Mercado, I. A. Baburin, D. M. Proserpio, B. Smit, *Proc. Natl. Acad. Sci.* **2018**, 115.
[3] K. M. Cheung, Y. Xiong, S. H. Pun, X. Zhuo, Q. Gong, X. Zeng, S. Su, Q. Miao, *Chem* **2023**, *9*, 2855-2868.
[4] K. Kawasumi, Q. Zhang, Y. Segawa, L. T. Scott, K. Itami, *Nat. Chem.* **2013**, *5*, 739-744.
[5] S. M. Elbert, O.T. A. Paine, T. Kirschbaum, M. P. Schuldt, F. Rominger, M. Mastalerz, **2024** *manuscript in preparation*.

Tuning Electron Transfer Coupling and Exchange Interaction in Bis-triarylamine Radical Cations and Dications by Bridge Electron Density

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To explore the influence of the electron density of the bridge connecting two redox centres on both the hole transfer and magnetic superexchange, a series of 2,7-fluorene bridged bis-triarylamine mono- and di-cations with varying bridge electron density was synthesized. By analysis of the intervalence charge-transfer bands of the mono-cations using the *Generalized Mulliken Hush* theory and VT-EPR spectroscopy of the di-cations the exchange and magnetic couplings were determined and analyzed. This series of molecules allows to correlate both forms of electronic communication with the energy of the optically accessible bridge state, suggesting a design guideline for both electronically and magnetically coupled organic compounds.

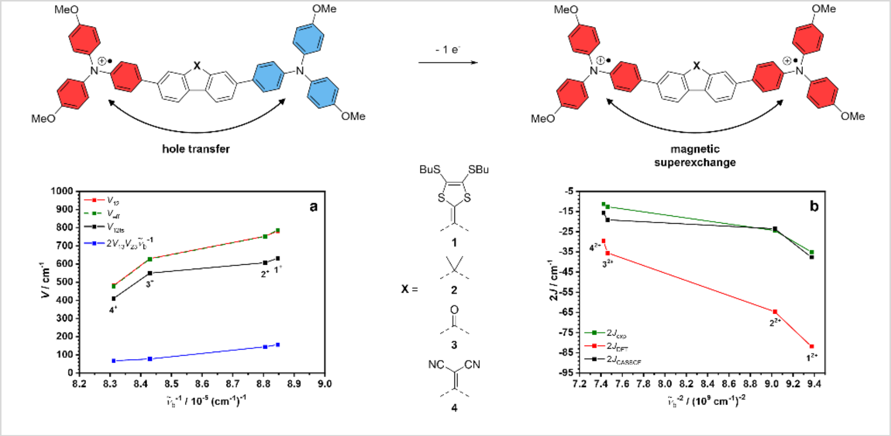

Figure 1: Model-systems **1** to **4**, a) electronic coupling *V* of the radical cations vs. inverse bridge state energy $\tilde{\nu}_b^{-1}$, b) magnetic exchange coupling 2*J* vs. inverse squared bridge state energy $\tilde{\nu}_b^{-2}$.

Switching It Up: Enhancing the Photochromic Behavior of Imines

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Molecules and materials comprised of dynamic-covalent imine bonds display a myriad of desirable properties including stimuli-responsiveness, recyclability, and effortless preparation, among others. One frequently overlooked property of imines is their photochromism. While the *E*/*Z* photoisomerism of arylimines has been known for decades, it has been unexplored relative to their azo-based counterparts. This is attributed to their suboptimal photoswitching properties (Figure 1a).[1] Inspired by these recent advancements in azo-based photoswitches[2] and the timeliness of light-controlled systems, we turned our attention to the relatively over-looked imine photoswitches.

We have overcome the previous limitations of imine-based photo-switches by replacing one of the phenyl rings with a heteroarene, affording a novel class of photoswitch, the aryliminopyrazoles (AIPs, Figure 1b).[3] Our findings open avenues for next-generation photoresponsive dynamic-covalent materials driven solely by these new photochromic linkages and we hope to impart light-responsiveness to existing imine-based materials.

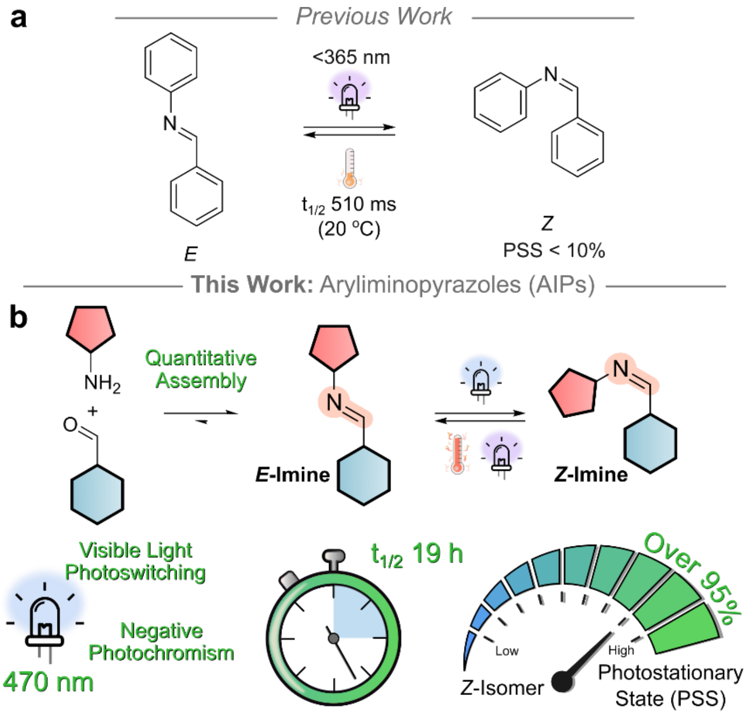

Figure 1: Overview of properties of a) previously reported imine photoswitches[1] and b) the improved (AIPs).[3]

References:

(1) Y. Luo, M. Utecht, J. Dokić, S. Korchak, H.-M M. Vieth, R. Haag, P. Saalfrank, *ChemPhysChem*, **2011**, *12*, 2311–2321.
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Synthesis of Chiral Pyrene-Based 1,4-Dithiins

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The incorporation of two sulfur atoms within a *π*-conjugated carbon scaffold makes 1,4-dithiins a special class of six-membered heterocyclic compounds of steadily growing interest.[1–3] Dithiins are known for their reversible redox properties to generate radical cations and thus are interesting for functional materials.[4,5] Furthermore, 1,4-dithiins typically adopt non-planar boat-conformations, which can be used to construct curved and sulfur-rich PAHs based on pyrene,[3] corannulene[6] or nanobelts.[2] However, chiral dithiin compounds are rarely encountered and, if so, their chiroptical investigations are very limited. Here we present the synthesis of several structurally-related pyrene-fused dithiins containing stereogenic centers on the core dithiin motif with a focus on tuning circular dichroism in respect to *g*-values depending on their connectivity.[7]

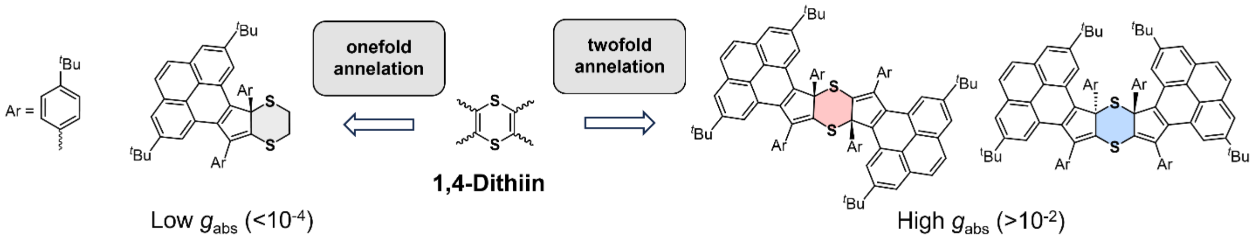

Figure 1: Chiral title compounds carrying the same pyrene-backbone, but with different connectivities to the dithiin core.

References:

[1] H. Jia, A. P. Häring, F. Berger, L. Zhang, T. Ritter, *J. Am. Chem. Soc.* **2021**, *143*, 7623.
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A Lateral Expansion Strategy for Molecular Spoked Wheels

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A lateral expansion strategy of molecular spoked wheels (MSWs) based on an *all*-phenylene backbone is a task that turned out to be challenging. The MSWs contain a central hub, six spokes and a rim that is formed by a six-fold *Yamamoto* coupling of the respective non-cyclized dodecabromo precursor. Attempts to prepare such compounds without flexible side groups at the spokes were unsuccessful, most probably due to an aggregation and accompanying oligomerization of the precursors during the cyclization. To overcome these problems, fluorene units are introduced at the spokes. These contain additional alkyl chains and lead to a curvature of the wheels. Quantum-chemical calculations using a geometric model and strain calculations predict their synthetic accessibility and subsequently these structures were synthesized with four and even six phenylene units at each edge of the hexagonal wheel. The resulting MSWs were characterized by spectroscopic methods and additionally some of them are visualized via scanning tunneling microscopy (STM).

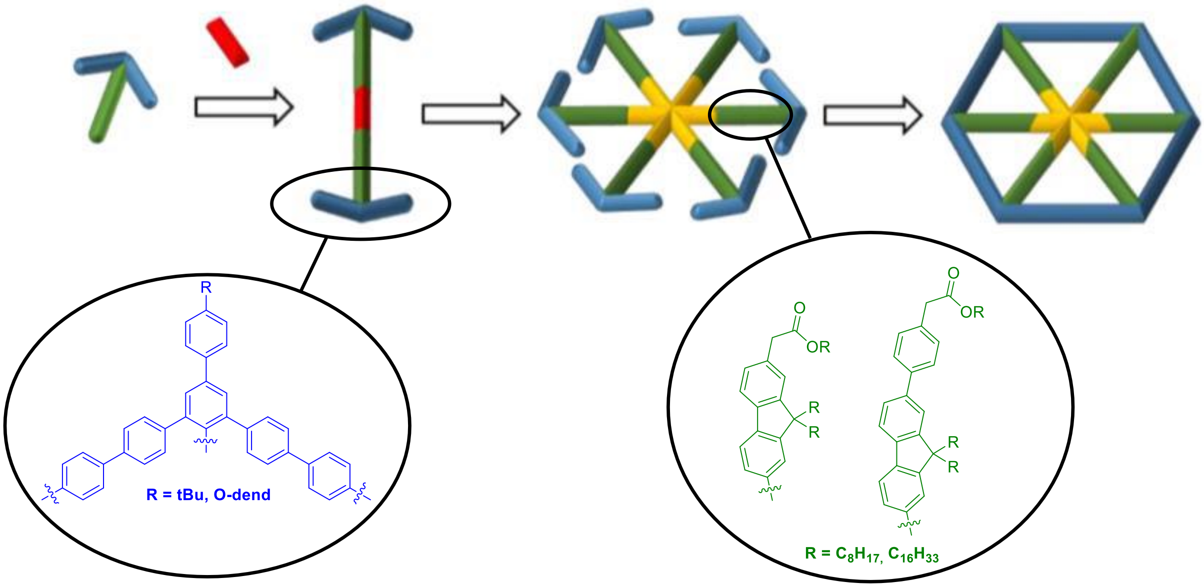

Figure 2: Schematic overview over the synthesis and enlargement of MSWs highlighting some of the key structural motifs.

Outstanding Chiroptical Properties of Conjugated Polygon-Shaped Macrocycles

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The increasing interest in conjugated carbon-based macrocyclic structures, induced by their promising photophysical properties, is strongly coupled to the development of new synthetic strategies. Recently, we reported the use of pseudo-*meta*[2.2]paracyclophanes (PCPs) as corner units. Their geometry, given by the substituents angle, allows the straight-forward assembly of unstrained macrocyclic systems, while the efficient electronic conjugation and chiral information are maintained.[1]

The acetylene homocoupling of enantiopure dialkyne pseudo-*meta* PCP allowed to isolate four enantiopure polygon-shaped structures in high yields (see below). Unprecedented high molar circular dichroism values for all-carbon structures were found reaching up to 1307 $\mathrm{Lmol^{-1}cm^{-1}}$.[1] In order to obtain bright circularly polarized emitters the 1,3-butadiyne linked library was heterocyclized to the 2,5-thienyl derivatives in high yields (see below).[2] The optical and chiroptical properties oft he two resulting libraries were analyzed and compared to each other. While the 1,3-butadiyne linked structures revealed through-space conjugation the 2,5-thienyl derivatives posses significantly higher quantum yields.[1,2]

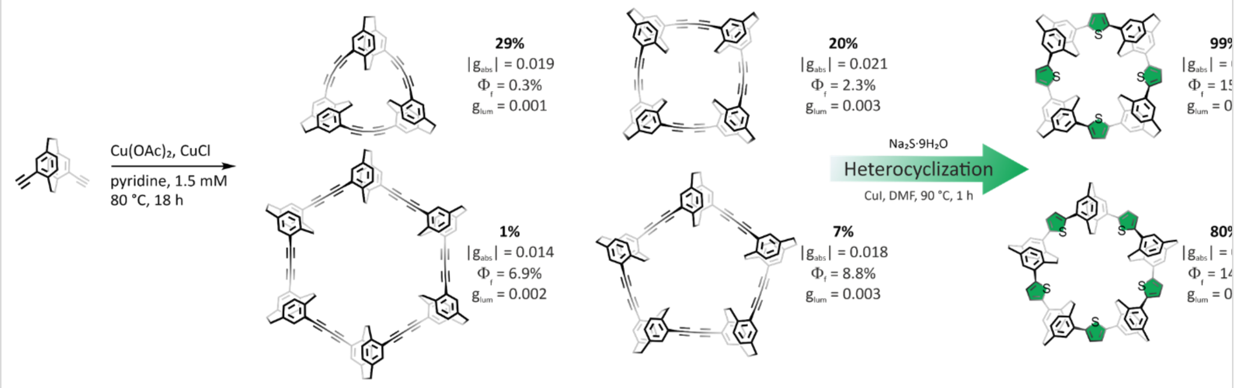

Figure: Synthesis and comparison of the polygon shaped 1,3-butadiyne and of the 2,5-thienyl linked pseudo-*meta* PCP macrocycles.

References:

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[2] C. Kress, E. Sidler, P. Downey, P. Zwick, O. Fuhr, D. Fenske, S. Bernhard, M. Mayor, *Chem. Eur. J.* **2024**, e202303798.

Supramolecular polymers as model systems for organic optoelectronics

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In organic optoelectronics, performances are determined by intrinsic molecular properties and emergent functions arising from supramolecular organization. A fundamental understanding of the underlying structure-assembly-property relationships is therefore crucial to define design principles for advanced materials. At the core of the presented research is the use of one-dimensional supramolecular assemblies as model systems for the study of the primary processes at the basis of optoelectronic materials, with the final goal of unlocking new opportunities in energy conversion technologies. In this context, long-lived triplets from singlet fission in pentacene-decorated helical supramolecular polymers and tunable emission from H-type assemblies of tetraphenylethylene monomers in optical nanocavities will be discussed.[1,2]

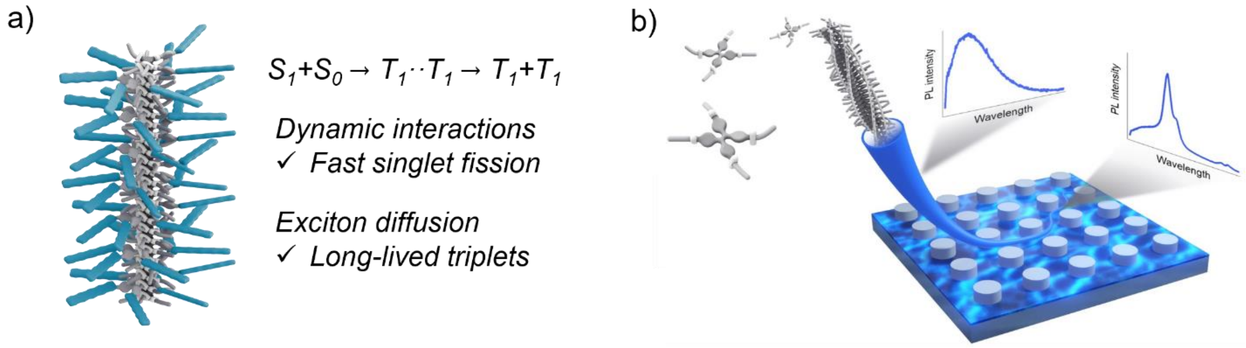

Figure 1: a) Singlet fission in pentacene-decorated supramolecular polymers. b) Tunable emission from stacked tetraphenylethylene assemblies in optical nanocavities.

References:

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Through-space charge transfer in anthracene-based emitters – a new paradigm for TADF molecules

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Molecules featuring hot excited states represent an interesting class of emitters capable of thermally activated delayed fluorescence (TADF).[1] Representatives for these emitters rely on a so-called hot exciton or hot exciplex mechanism.[2] Both emission pathways have several characteristics in common: they rely on charge-transfer excited states, exhibit acceptable oscillator strengths, and are reported to exhibit extremely fast delayed fluorescence, almost indistinguishable from the prompt component.

In my work, I will compare donor-acceptor functionalized anthracenes that feature either hot exciton or hot exciplex emission, and I will explain why hot exciplexes show higher photoluminescence quantum yields than hot exciton molecules.[3] After optimization of the donor and acceptor strength (see Figure), I will present our most powerful emitter in an OLED with efficiency beyond the spin-statistical limit.

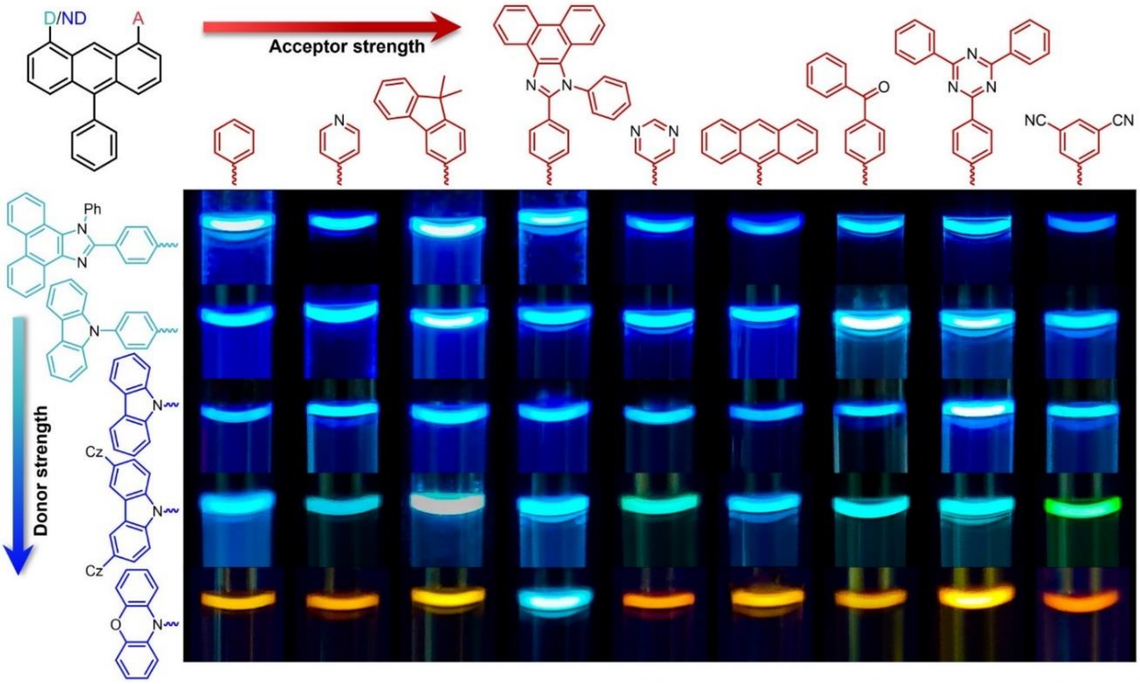

Figure 1: Optimization matrix of anthracene-based hot exciplex emitters.

References:

[1] Y. Xu, P. Xu, D. Hu, Y. Ma, *Chem Soc Rev* **2021**, *50*, 1030–1069.
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Non-Fullerene Acceptors in Organic Solar Cells – Some new Insights

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In recent years, non-fullerene acceptors (NFAs) have attracted a lot of attention, because organic solar cells (OSC) based on NFAs have better performance than previous PCBM-based (soluble fullerene) devices. Despite of their excellent performance in OSCs, sometimes only irreversible reduction in cyclic voltammetry (CV) is reported for some of the most reliable NFAs, whereas the origin behind this remains unclear.

In this paper, we investigate the potential impact of this issue on device performance, in particular long-term stability. We use a combination of mass spectrometry (MS) and CV.

Indenoannulated Tridecacyclene: An All-Carbon Seven-Stage Redox-Amphoter

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The embedding of 5-membered rings into a polycyclic aromatic hydrocarbon (PAH) facilitates electron uptake through the formation of aromatic cyclopentadienyl anion-like subunits.[1] Similarly, 8-membered cyclooctatetraene carbocycles impart redox activity by aromatic stabilization of the respective 6 π electron dication and 10 π electron dianion.[2] By indenoannulation of the tridecacyclene scaffold,[3] we strategically combine an octagonal and multiple pentagonal rings to yield a highly redox-active all-carbon scaffold (Figure 1).[4]

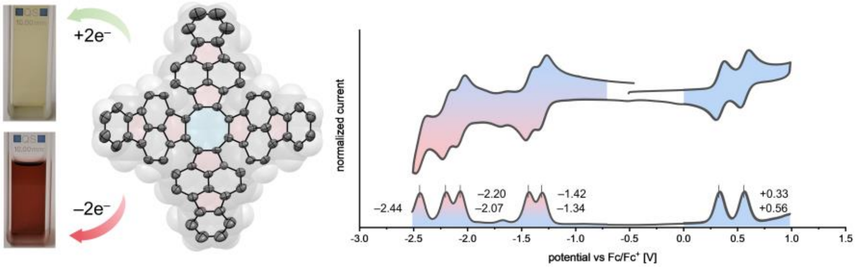

Figure 1: X-ray crystal structure and redox properties of indenoannulated tridecacyclene.

The saddle-shaped PAH undergoes seven reversible redox events comprising five reductions and two oxidations under electrochemical conditions. The properties of the charged species were comprehensively studied spectroscopically and supported by theory.

References:

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Conformationally Regulated Molecular Conductance Switching in Arylene-Bridged Bis(Triarylamines)

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Charge transport on the nanoscale has its own intricacies and offers unique opportunities when compared to the macroscopic scale. Of particular interest for the construction of basic components for memory and logic devices are conductance switches, which offer two or more different states.[1]

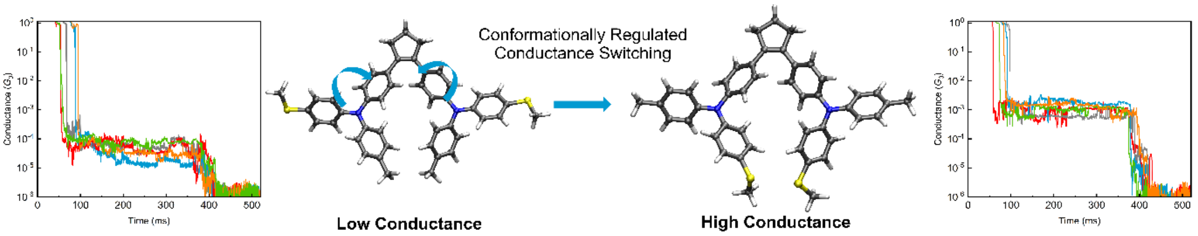

Figure 1: Two different molecular conformations with different $S\cdots S$ distances (middle) with corresponding selected single traces, showing low (left) and high conductance (right).

We have devised and synthesized anchor-group modified bis(triarylamines), as exemplarily shown in Figure 1, which feature different degrees of rotational flexibility encoded in their molecular backbone and compared their molecular conductance characteristics. The latter were measured by means of a custom-built scanning tunneling microscope, according to an established design and protocol.[2] We present evidence for a conformationally regulated conductance dualism in molecular structures of appropriate rotational flexibility, relying on different charge transport pathways across the molecular junction.

References:

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[2] (a) L. Venkataraman, J. E. Klare, I. W. Tam, C. Nuckolls, M. S. Hybertsen, M. L. Steigerwald, *Nano. Lett.* **2006**, *6*, 485-462; (b) L. Venkataraman, J. E. Klare, C. Nuckolls, M. S. Hybertsen, M. L. Steigerwald, *Nature* **2006**, *442*, 904-907. (c) A. Mang, N. Rotthowe, K. Beltako, M. Linseis, F. Pauly, R. F. Winter, *Nanoscale* , **2023**, *15*, 5305-5316.

Multilayer Helical Nanographenes with Layer-Dependent Chiroptical Properties

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Helical nanographenes (NGs) have emerged as a captivating class, distinguished by their inherent chirality and exotic chiroptical properties. With the incorporation of [n]helicene units into NGs, a variety of helical NGs with diverse multilayer topologies have been reported and considered to be the impetus for the development of novel tailor-made chiroptical materials with high circularly polarized luminescence (CPL) brightness.

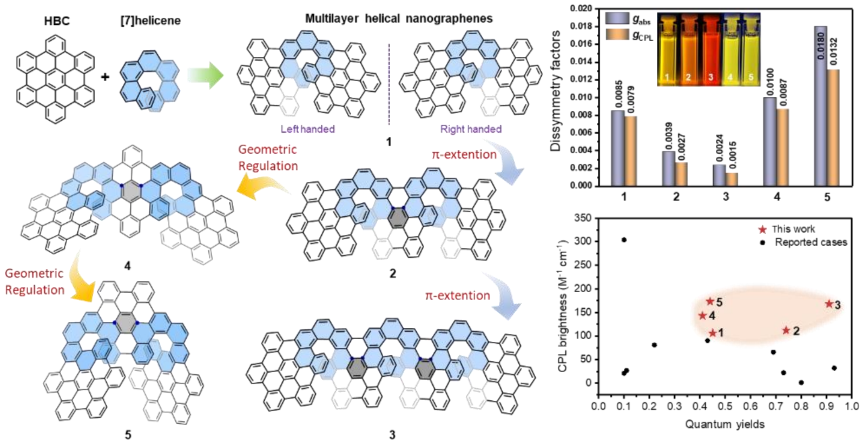

Figure 1: Helical nanographenes **1**-**5** with multilayer topologies and layer-dependent chiroptical properties.

Herein, we demonstrated the modular synthetic strategy to construct a series of novel helical NGs (**1**-**5**) with bilayer, trilayer, and tetralayer structures. The resultant NGs exhibit excellent circular dichroism (CD) and CPL responses with high dissymmetry factors and CPL brightness, rendering them promising candidates for CPL emitters. In addition, we tried to understand the intricate interplay between the multilayer chiral structure and chiroptical properties, rendering the development of chiral materials with modulated CPL properties.

References:

[1] W. Niu, et al., *J. Am. Chem. Soc.* **2023**, *145*, 26824-26832
[2] W. Niu,* et al., *Angew. Chem. Int. Ed.* **2024**, e202319874.

Molecular Engineering of Helically Chiral Functional Molecules: Materials for Next Generation (Opto)electronics

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In the era of miniaturization—aiming to build ever smaller and more efficient optical, electronic, and mechanical devices—there is an increasing demand for multifunctional materials, which can respond to multiple external stimuli simultaneously. To address this challenge, we aim to explore ways to custom-build multifunctional molecules by taking advantage of chirality—a property of molecules related to their symmetry. The introduction of chirality in π-conjugated organic compounds gives rise to properties such as absorption and emission of circularly polarized light, magneto-chiral anisotropy, and spin-selective charge transport, which enable the conceptualization of novel functions and applications.

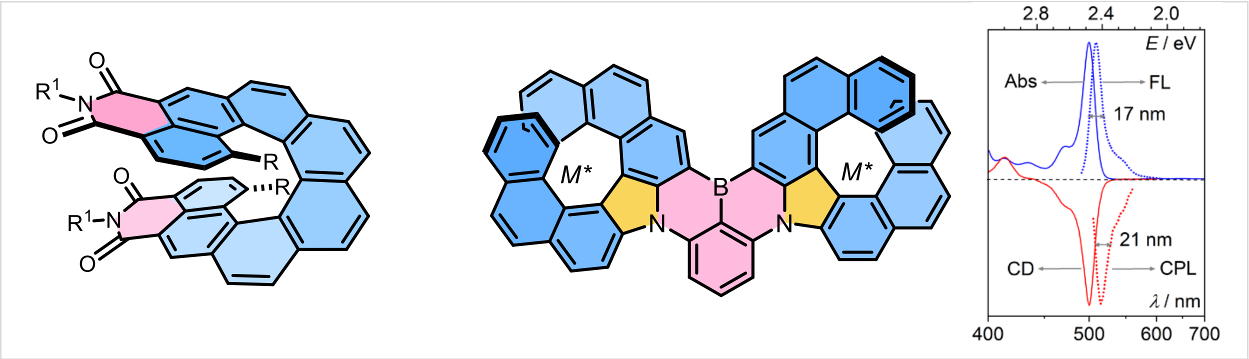

Figure 1: Helicene based functional chiral molecules and narrowband FL & CPL from helicenes.

My presentation will focus on—1. A novel class of [*n*]helicene diimides features through-bond and through-space interactions. 2. Unprecedentedly narrowband fluorescence (FL) and circularly polarized luminescence (CPL) from 1,4-B,N-embedded helicenes.

References:

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[2] *Angew. Chem. Int. Ed.* **2021**, *60,* 23656–23660.
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[6] *Chem. Eur. J.* **2019**, *25*, 16241–16245.

Molecular conductance of diaryl amine capped carbon-bridged oligo(phenylene vinylene)s

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Molecules featuring topological edge states, like unpaired spins localized at the molecular termini, are known for their increasing molecular conductance as a function of the number of bridging repeating units[1]. This poses an exception to the universal rule of conductance decay in respect to molecule length, rendering them excellent candidates for the use as molecular wires by diminishing and even reversing electrical signal loss.

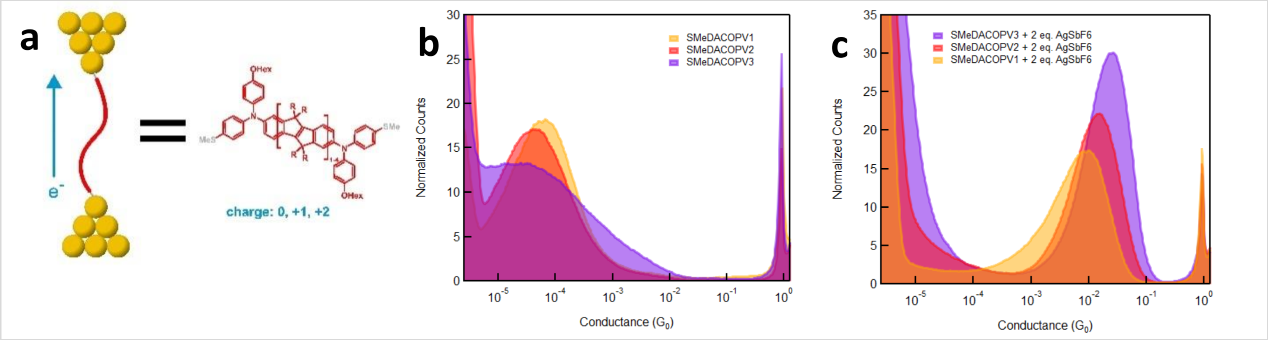

Figure 1: Schematic representation of the employed STM-BJ method (a). Conductance histograms of the neutral series (b) the oxidized series (c).

Diaryl amine-capped carbon-bridged oligo(phenylene vinylene)s express excellent charge transport characteristics[2] and offer two redox centers to create topological states. We investigate the molecular conductance of a series of 1-3 repeating units in their neutral and cationic states *via* STM break junction, revealing notable conductance values for neutral molecules of these dimensions, as well as the intended reverse conductance decay for the oxidized species.

References:

[1] L. Venkataraman, *et al.*, *Nat. Chem.* **2022**, *14*, 1061-1067.
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Added Value of Circular Dichroism for Studying Charge Transfer Excitons in Photoactive Organic Thin Films

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Organic semiconductors have emerged as promising materials for various optoelectronic applications due to their unique properties and easy adjustability. For such optoelectronic devices, however, it is essential to acquire a fundamental understanding of the underlying processes and mechanisms such as the generation, transport and nature of excitons. *N*-alkyl anilino squaraines are prototypical materials for such applications, featuring distinctive double humped absorption spectra.[1] To explain this absorption pattern by theoretical modeling, two different approaches have been used so far. The first theoretical model is an essential state model which uses intermolecular Frenkel excitons in combination with intermolecular charge transfer excitons.[2,3] The other suitable model, however, assumes an ensemble of aggregates with intermolecular dipole–dipole resonance interactions and structural disorder in the thin film to describe the unpolarized absorbance spectrum.[4]

Here, we investigate the structure-correlated excitonic properties in photoactive thin-film semiconductors for optoelectronics by comparing non-chiral nBSQ and nOSQ to two new structurally related chiral anilino squaraines. Substitution of only one *n*-alkyl side chain with an enantiomerically pure citronellyl-derived residue ensures the analogy to the corresponding *n*-alkylated compounds. The presence of the same double hump absorption features allows comparison with the *n*-alkyl derivatives, while an emerging excitonic chiral dichroism (CD) simultaneously enables investigation by Mueller matrix polarimetry. These dyes are thus predestined to provide a deeper insight into the nature of excitonic transitions between aggregated squaraine molecules.

References:

[1] J. Zablocki et al., *J. Phys. Chem. C* **2020** ,*124*, 41, 22721–22732.
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[4] F. Balzer et al., *J. Phys. Chem. C* **2022**, *126*, 32, 13802–13813.

Redox-Switchable Aromaticity in a Helically Extended Indeno[2,1-*c*]fluorene

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Antiaromaticity is a fascinating property that has attracted not only significant fundamental interest but is also increasingly relevant in different applications, in particular organic (opto)electronics. However, designing systems in which (anti)aromaticity can be judiciously and reversibly switched ON and OFF remains challenging. Herein, we report a helicene featuring an indenofluorene[1]-bridged bisthioxanthylidene[2] as a novel switch wherein a simultaneous two-electron (electro)chemical redox process allows highly reversible modulation of its (anti)aromatic character. Specifically, the two thioxanthylidene rotors, attached to the initially aromatic indenofluorene scaffold via overcrowded alkenes, adopt an anti-folded structure, which upon oxidation convert to singly bonded, twisted conformations. This is not only associated with significant (chir)optical changes but importantly also results in formation of the fully conjugated, formally antiaromatic *as*-indacene motif in the helical core of the switch. This process proceeds without the formation of radical cation intermediates and thus enables highly reversible switching of molecular geometry, aromaticity, absorbance and chiral expression under ambient conditions.

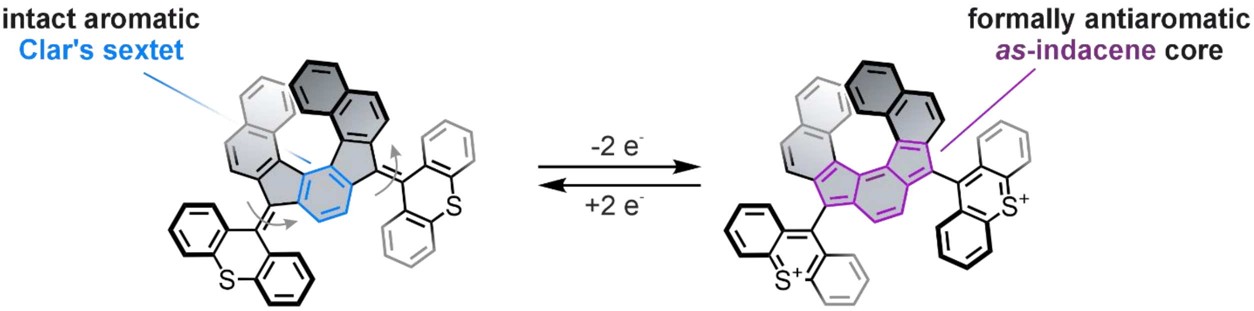

Figure 1: General redox switching scheme of the extended helically chiral indeno[2,1-c]fluorene.

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Supramolecular DNA Architectures with Chromophores

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The helical structure of DNA, well defined stacking distances and sequence recognition make DNA very attractive as structural scaffold[1,2] for the sequence-defined supramolecular architectures of two chromophores[3,4] and of different chiralities.[5] Completely self-assembled supramolecular DNA architecture are hierarchically ordered and the DNA template controls not only the binding but also the energy transport properties (Figure 1).[6-9] Using click chemistry, the supramolecular DNA-based chromophore arrangements can be converted into covalent oligomers with full sequence control.

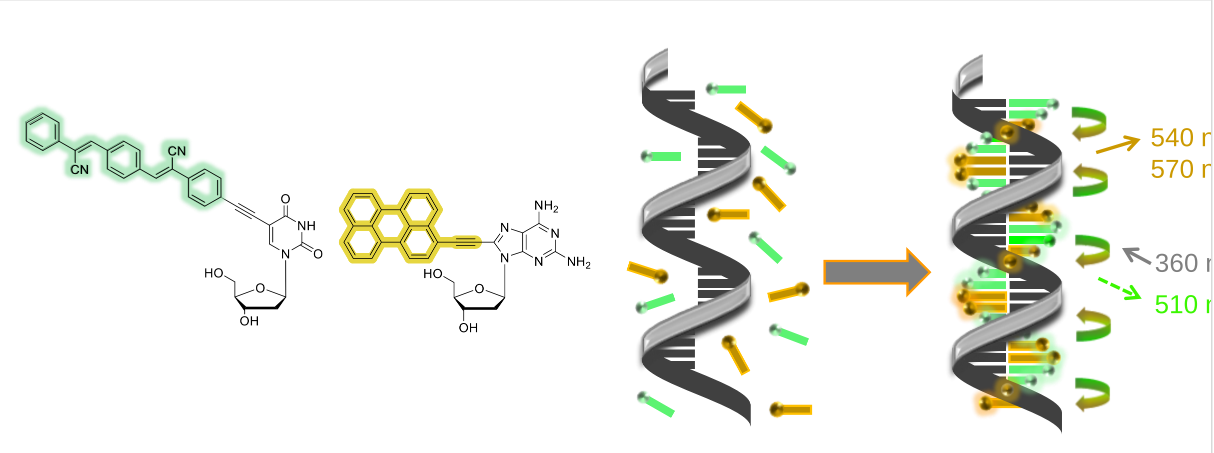

Figure 1: Sequence-selective supramolecular DNA architecture with two different chromophores

References

[1] Account: P. Ensslen, H.-A. Wagenknecht, *Acc. Chem. Res.* **2015**, *48*, 2724-2733.
[2] P. Ensslen, Y. Fritz, H.-A. Wagenknecht, *Org. Biomol. Chem.* **2015**, *13*, 487-492.
[3] R. Hofsäß, S. Sinn, F. Biedermann, H.-A. Wagenknecht, *Chem. Eur. J.* **2018**, *24*, 16257-16261.
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[8] H. Ucar, H.-A. Wagenknecht, *Chem. Sci.* **2021**, *12*, 10048-10053.
[9] H. Ucar, H.-A. Wagenknecht, *Chem. Commun.* **2022**, *58*, 6437–6440.

Synthesis of Electronic Delocalized Möbius Belt

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The Möbius strip, with only one non-orientable surface, was first discovered by August Ferdinand Möbius and Johann Benedict Listing independently in 1858. Due to its captivating topological structure, Möbius strip has garnered significant attention from mathematicians, engineers, and chemists. Herein, we summary two synthetic strategies towards molecular Möbius belt. Strategy I involves introducing a twist ($T_W = 1$) into a normal carbon nanobelt (CNB),[1] while Strategy II focuses on integrating a writhe ($W_r = 1$), essentially a helical component, within a normal belt.[2] In this work, we report a successful synthesis of a double-stranded Möbius belt using Strategy II. It exhibits a zigzag molecular backbone featuring 14 linearly fused heteroarene, which is the extended version of Herges's Möbius annulene. The helical moiety in Möbius belt not only significantly alleviates the strain energy by winding the rigid backbone, but also precisely controls the chirality of Möbius belt compared to those formed by Strategy I. The studies with NMR spectroscopy and DFT calculations provide evidence that Möbius belt exhibits a weak global electron communication.

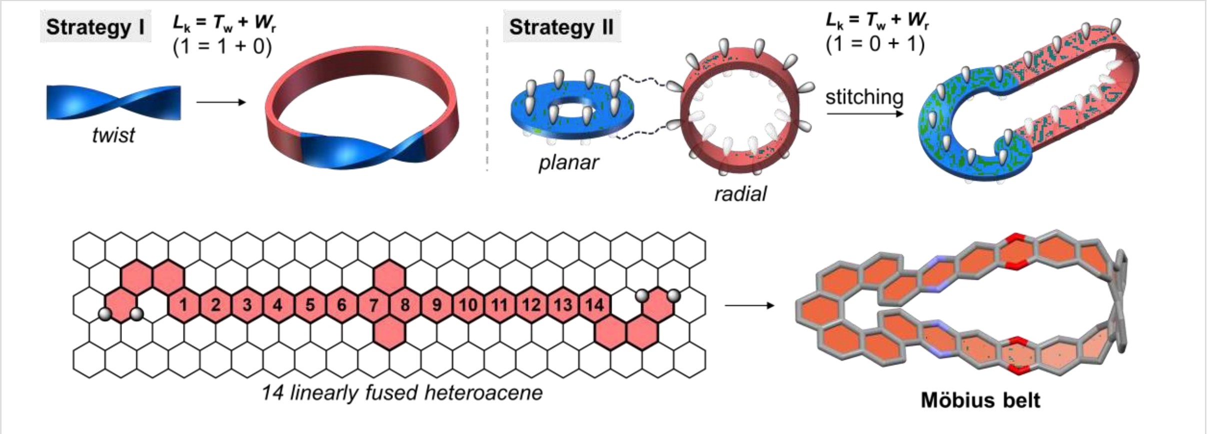

Figure 1: Two synthetic strategies towards molecular Möbius belt, and structure of Möbius belt.

References:

[1] Y. Segawa, T. Watanabe, K. Yamanoue, M. Kuwayama, K. Watanabe, J. Pirillo, Y. Hijikata, K. Itami, *Nat. Synth.* **2022**, *1*, 535-541.

[2] D. Ajami, O. Oeckler, A. Simon, R. Herges, *Nature* **2003**, *426*, 819-821.

Posters

Synthesis of Novel Proline derived Squaraines for Applications in Optoelectronic Devices

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Chiral aggregates are still in demand today as materials for optoelectronic components in the field of sensor technology. Squaraine molecules, in particular, hold considerable interest in this regard. Aggregates of homochiral proline-based squaraines (ProSQ's) have been shown to have a particularly strong CD effect.[1] Moreover, aggregation can be influenced by many factors, especially the functionalities of the molecules play a major role in influencing intermolecular packing effects. Introducing aryl units to modify the ProSQ's could facilitate improved aggregation by enhancing π-π stacking interactions. This, in turn, has the potential to amplify the CD effect.

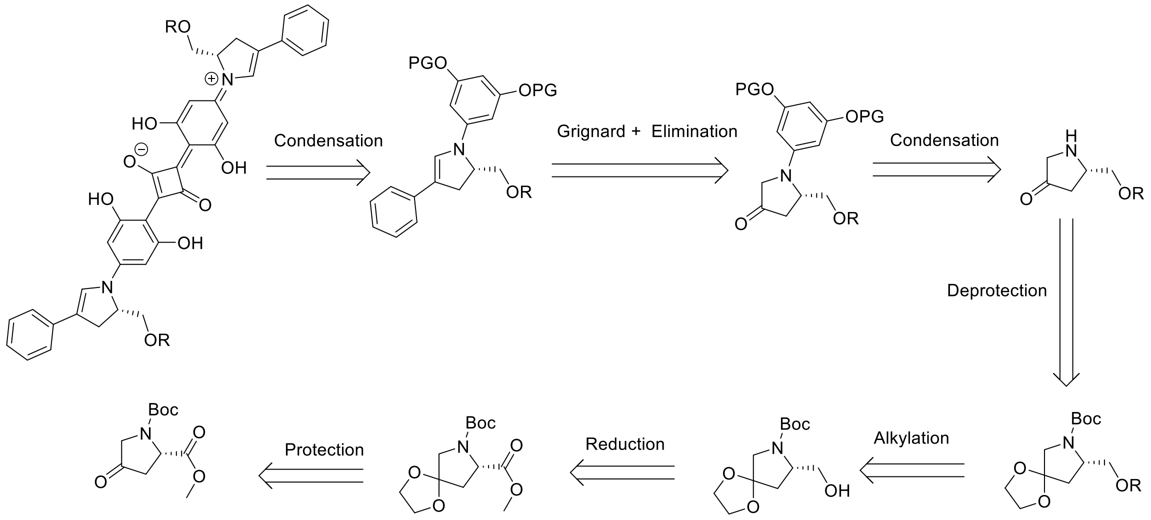

Figure 1: Retrosynthetic approach of a new proline-derived Squaraine.

A new idea on how to obtain aryl-substituted proline derivatives is shown in Fig. 1, with the key step of a Grignard reaction. With this sequence in particular, there is potential for accessibility to various other derivatives via different Grignard reactions.

References:

[1] M. Schulz, J. Zablocki, O. S. Abdullaeva, S. Brück, F. Balzer, A. Lützen, O. Arteaga, M. Schiek, *Nature communications* **2018**, *9*, 2413.

B,N-Embedded Helicenes with Narrowband Circularly Polarized Luminescence

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Extended aromatic systems bearing 1,4-azaborine subunits have been studied in recent years due to their photochemical properties and their applications as OLED materials; the azaborine-based design allows for a remarkably narrow-band emission and for high quantum efficiency. We further extended the scope of these systems by functionalizing B,N-embedded polycyclic aromatic systems with helically chiral subunits, thus resulting in molecules capable of narrowband circularly polarized luminescence (CPL). By rigidification of the molecular backbone, unprecedented narrowband CPL for a small molecule was achieved.

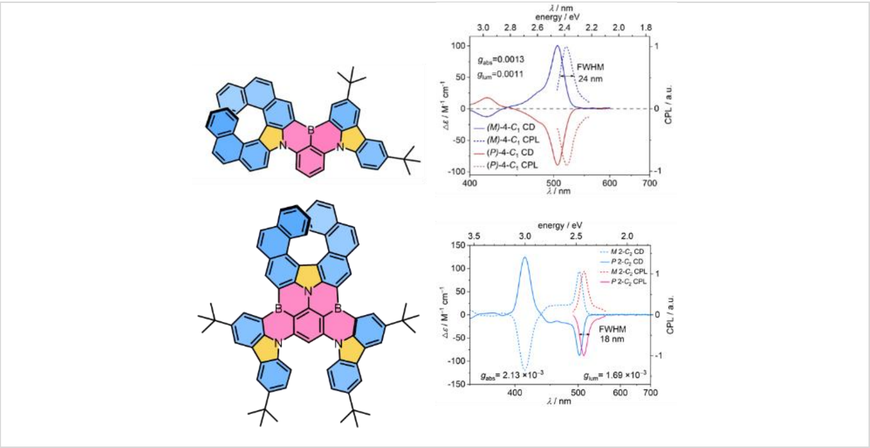

Figure 1: B,N-embedded CPL emitters, featuring subunits with well-defined chirality within the π system, and their CD/CPL spectra

References:

[1] F. Zhang, F. Rauch, A. Swain, T. B. Marder, P. Ravat, *Angew. Chem., Int. Ed.*, **2023**, 62, e202218965

Tailoring Peptide Self-Assembly with Electron Donor Functionalization Towards Formation of Vesicles, Helical Ribbons, and Fibers

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We present the synthesis of novel tripeptides functionalized with triarylamine-based donor moieties and their self-assembly in aqueous solutions. After successful synthesis of the amino acids decorated with donor moieties (Figure 1, red), solid-phase peptide synthesis enabled the isolation of a series of tripeptides with different *N*-terminal protection groups (Figure 1, blue). In the series of Fmoc-protected peptides, electron microscopy images revealed that the incorporation of the triphenylamine (TPA)-substituent induced fiber formation, while the bridged *N*-heterotriangulene (*N*-HTA) yielded helical ribbons. For the unprotected peptides, dynamic light scattering measurements detected vesicles with diameters of up to 300 nm, which were visualized by SEM. For the bridged-donor decorated peptide, irradiation with UV-light led to decomposition of the vesicles, presumably due to photochemically induced oxidation of the nitrogen center, which is enabled by a lower oxidation potential compared to parent triphenylamine.[1] Hence, this tripeptide shows promise for cargo transportation in aqueous media.

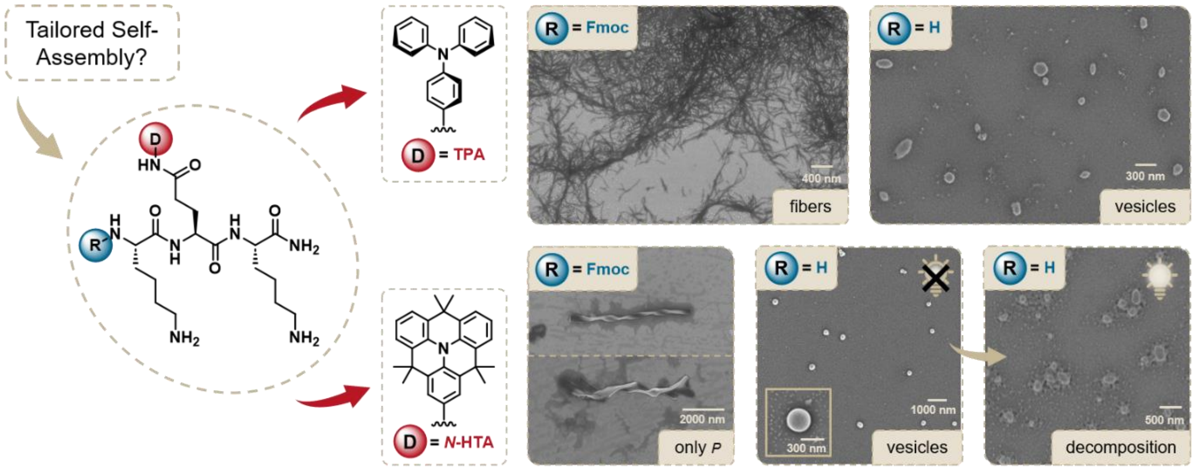

Figure 1: Decoration of tripeptide with distinct triarylamine based donor moieties leads to tailored self-assembly.

References:
[1] N. Hammer, T. A. Schaub, U. Meinhardt, M. Kivala, *Chem. Rec.* **2015**, *15*, 1119-1131.

Tailored Synthesis of Oligo(Arylene Ethynylene)s to Tune Their Optoelectrical Properties

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Sequence-defined conjugated molecules are of interest in materials science, in particular to gain insight into structure-property relationships.[1] Our group showed sequence-definition in uniform pentamers of oligo(phenylene ethynylene) by applying stepwise Sonogashira cross-coupling reactions.[2] To streamline the synthetic process, an iterative strategy consisting of a decarboxylative cross-coupling and a saponification of an alkynyl carboxylic ester was established subsequently.[3] To this point, we can customize the oligomers efficiently and have full control of each repeating unit. Hence, we synthesized molecules of oligo(arylene ethynylene) patterns towards optoelectronic properties assisted by quantum mechanical calculations and report their modelling guided synthesis and properties.

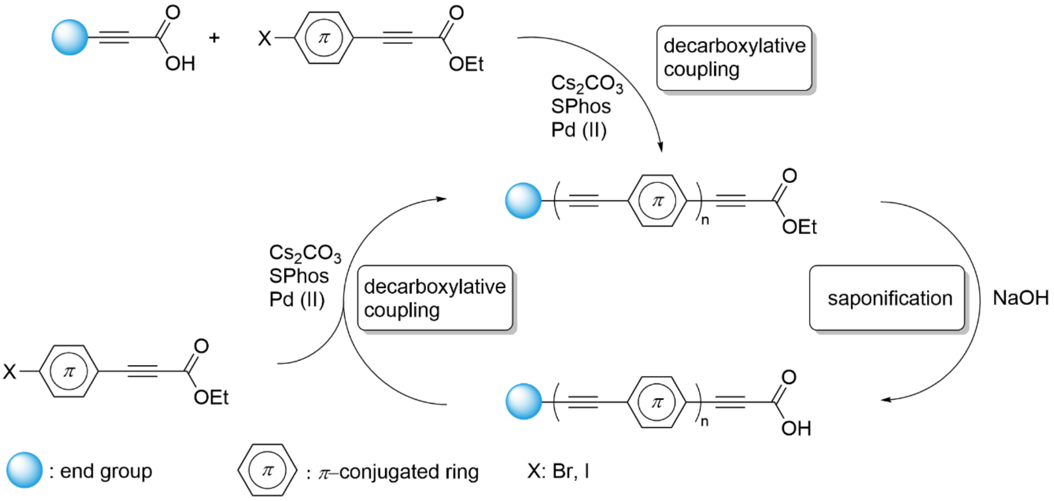

Figure 3: Schematic illustration of sequence-defined synthesis towards uniform OAEs based on a two-step iteration cycle of a decarboxylative cross-coupling and a saponification of an alkynyl carboxylic ester.[1]

References:

[1] a) H. Yu, S. Li, K. E. Schwieter *et al*, *J. Am. Chem. Soc.* **2020**, *142*, 10, 4852-4861. b) C. Xu, C. He, N. Li *et al*, *Nat. Commun.* **2021**, *12*, 5853. c) H. Xu, S. Ye, R. Zhao, D. S. Seferos, *Angew. Chem. Int. Ed.* **2022**, *61*, e202210340. d) H. A. Mills, S. Rahman, R. Zigelstein *et al*, *J. Am. Chem. Soc.* **2023**, *145*, 10, 23519-23526.

[2] R. V. Schneider, K. A. Waibel, A. P. Arndt *et al*, *Sci. Rep.* **2018**, *8*, 17483.

[3] D. Hahn, R. V. Schneider, E. Foitzik, M. A. Meier, *Macromol. Rapid Commun.* **2021**, *42*, 2000735.

Investigation of the synthesis of a large acene precursor

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Acenes are polycyclic aromatic hydrocarbons (PAHs) consisting of linearly condensed benzene units. In comparison to their topological isomeric PAHs, acenes show up the smallest HOMO-LUMO gap. Based on the resulting, excellent properties, stabilized derivatives up to pentacene have been successfully applied as organic functional materials in electronic devices. Pushing the limits in synthesis of longer, unsubstituted acenes and their optical characterization gives further insight into their intriguing electronic structure.[1]

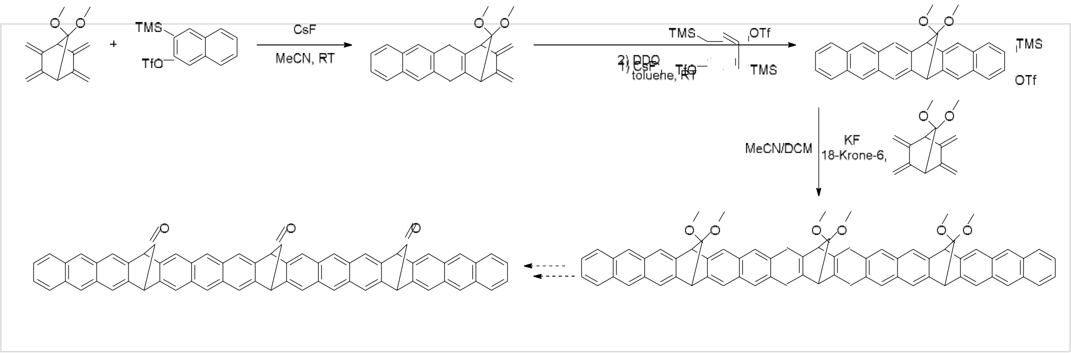

Figure 1: Synthesis of the [15]-acene monoketone bridged photoprecursor.

Due to their high reactivity, making use of sophisticated synthetic strategies and isolation techniques is inevitable in acene chemistry. In the present project, a Diels-Alder sequence starting from a dimethoxy-acetal-bridged bisdiene and leading to a potential photoprecursor of the so far unknown [15]-acene is being investigated.[2]

References:

[1] C. Tönshoff, H. F. Bettinger, *Chem.Eur.J.* **2021**, *27*, 3193–3212.
[2] A. Jancarik, G. Levet, A. Gourdon, *Chem.Eur.J.* **2019**, *25*, 2366– 2374.

Donor-Acceptor-Dyads with ^{15}N-labeled Triarylamine-Donor for Investigations of the Magnetic Field Dependent Spin Interconversion

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One main driving force behind spin interconversion in charge-separated states of organic bridged donor-acceptor compounds is the hyperfine interaction between radical electrons and the nuclei.[1, 2] Therefore, the ^{14}N isotope in the triarylamine donor was replaced by the ^{15}N isotope to study the resulting effects on spin interconversion. This was achieved by transient spectroscopy experiments in a tunable external magnetic field.

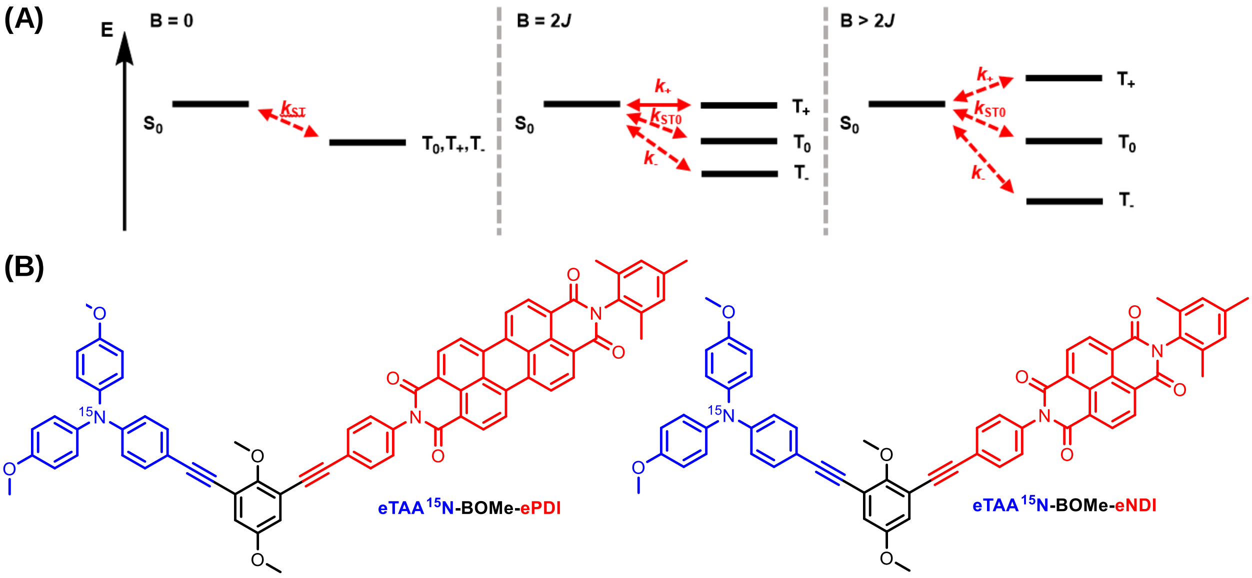

Figure 1: Magnetic field dependency of spin interconversion resulting from *Zeeman*-splitting in an external magnetic field **(A)** and investigated ^{15}N-labeled compounds **(B)**.

References:

[1] U. E. Steiner, T. Ulrich, *Chem. Rev.* **1989**, *89*, 51-147.
[2] B. Brocklehurst, *Chem. Soc. Rev.* **2002**, *31*, 301-311.

Chiroptical properties of axially chiral indolenine merocyanine dimers with varying acceptors

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Axially chiral indolenine based squaraine dyes were recently shown to exhibit pronounced electronic circular dichroism (ECD) signals ($\Delta\varepsilon$ up to ca 1500 M^{-1} cm^{-1}).[1] Based on these studies, merocyanine dimers with the same configuration determining axially chiral indolenine donor but with varying acceptor units were synthesised. Electro-optical absorption measurements revealed differences in the electronic structures of the dyes, where stronger electron-withdrawing acceptors led to a more cyanine-like character, while weaker acceptors resulted in a more polyene-like behavior. These properties had a significant influence on the ECD spectra, as the chiroptical quantities were enhanced in merocyanines at the cyanine limit compared to polyene-like compounds. This was traced back to the weaker spectral overlap of negative and positive signals in the ECD couplet for chromophores with narrow bandwidths.

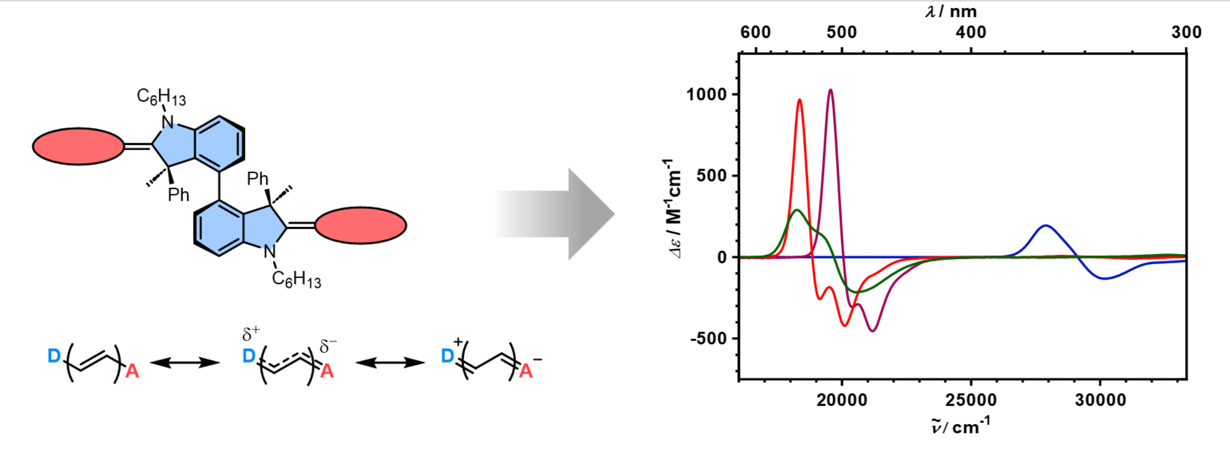

Figure 1: Axially chiral merocyanine dimers and their ECD spectra.

References:

[1] E. Freytag, M. Holzapfel, A. Swain, G. Bringmann, M. Stolte, F. Würthner, C. Lambert, *Chem. Sci.* **2022**, *13*, 12229-12238.

The Delayed Box: Biphenyl-bisimide Cyclophane, a Supramolecular Nano–environment for Efficient Generation of Delayed Fluorescence

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The burgeoning field of host-guest chemistry recently created immense attention in supramolecular chemistry due to their strong binding affinity and selectivity. Moreover, cyclophane hosts recently started blossoming due to their unique molecular design and functional relevance in sensing and catalysis. However, triplet-induced functional properties are still unknown in this scientific realm and remain a holy grail. In this context, we propose a strategy for efficient delayed fluorescence emission in a dilute solution state using a non-covalent approach via supramolecular nano–environment formation. We aim to create supramolecular nanocavity for triplet exciton stabilization by reducing vibrational dissipation and lowering the singlet-triplet energy gap for efficient delayed fluorescence emission. We elegantly entrench the design to alleviate the scenario using a novel small biphenyl bisimide-derived cyclophane, an electron-deficient and efficient triplet-generating host. We intend to form an emissive charge-transfer (CT) state close to the triplet level of the biphenyl bisimide upon encapsulating carbazole-derived guest inside the nanocavity of cyclophane. The experimental results of host-guest studies manifest high association constants up to 10^4 M^{-1}, which help in strong inclusion complex formation, prerequisites for emissive CT state evolution, and triplet-state stabilization in a diluted solution. According to our hypothesis, we realize tunable delayed fluorescence emission from carbazole-encapsulated biphenyl bisimide cyclophane in methylcyclohexane carbon tetrachloride solution via non-covalent supramolecular strategy with significantly high quantum yield (QY) of up to 15.6 % for the first time in solution. Further crystal structure analysis and solid-state photophysical study validate our hypothesis and elucidate the delayed fluorescence emission mechanism.

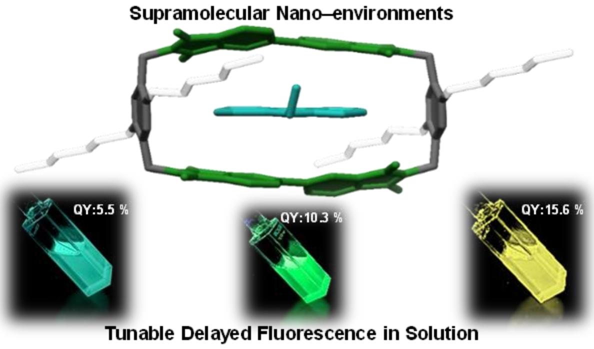

Figure 1: Single-crystal X-ray analysis of the host-guest complex and tunable delayed fluorescence of the host-guest complexes in MCH/CCl_4 (1:3) solvent mixture in an inert atmosphere under 365 nm UV light.

References:

[1] H. Uoyama, K. Goushi, K. Shizu, H. Nomura, C. Adachi, *Nature* **2012,** *492*, 234–238.
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Magnetic field dependent fluorescence in donor-acceptor-dyads

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Thermally activated delayed fluorescence in donor-acceptor-compounds can be used to construct highly efficient OLEDs.[1] By increasing the distance between both moieties electron transfer towards long lived charge separated states can be achieved, giving rise to a magnetic field dependent delayed fluorescence after endothermic charge recombination.[2] This fluorescence was studied by stationary and transient (fs to ns) spectroscopic experiments in the presence and absence of an external magnetic field to investigate the underlying electron transfer processes.

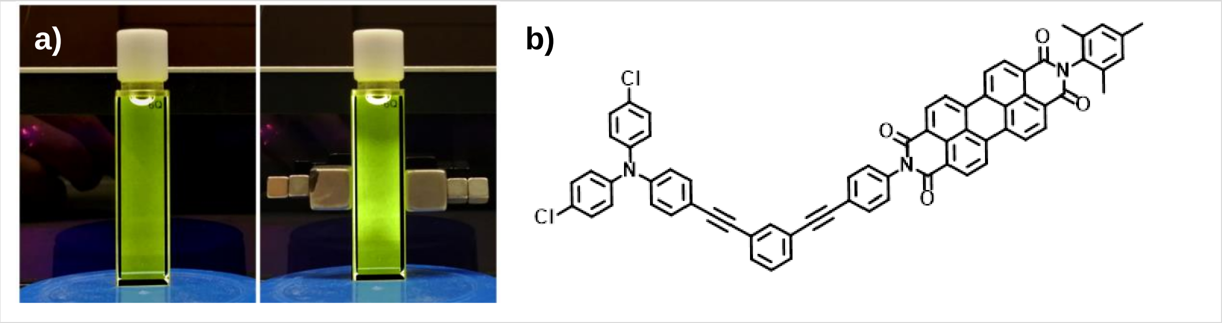

Figure 1: a) Increased fluorescence in an external magnetic field (right) produced by small permanent magnets and fluorescence without an external magnetic field (left) and b) molecular structure of the investigated compound.

References:

[1] P. Data, Y. Takeda, *Chem. Asian J.* **2019**, *14*, 1613-1636.
[2] J. T. Buck, T. Mani, *J. Am. Chem. Soc.* **2020**, *142*, 20691-20700.

Synthesis of π-Conjugated Oligomers Empowered by Sustainable Chemistry: Utilizing the Potential of Kolliphor® EL as an Eco-Friendly Emulsifier

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Synthesizing *π*-conjugated oligomers with optical properties for optoelectronic devices remains a top priority, as the demand for new electronic devices continues to grow. By incorporating chiral materials into OLEDs, it is possible to achieve direct circularly polarized light (CPL) emission, which enhances device performance by improving external quantum efficiency and thus reducing energy loss.

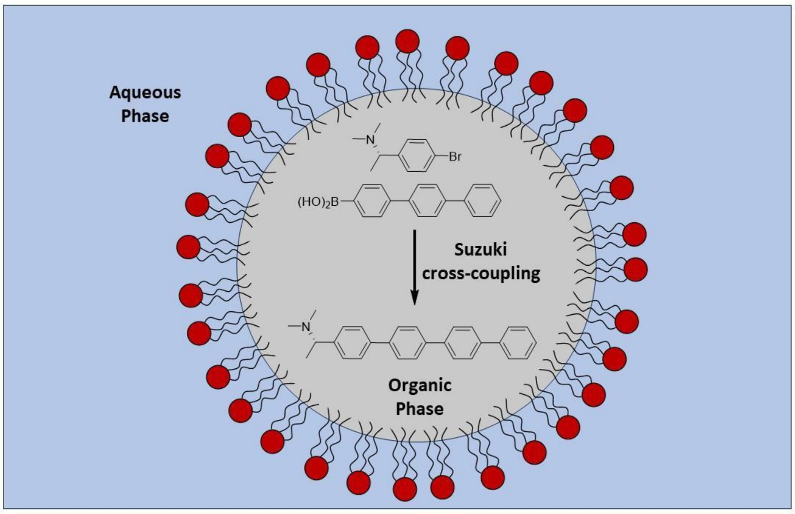

Figure 1: Schematic Representation of Micelle-Encapsulated Suzuki Cross-Coupling Reaction.

Utilizing non-ionic surfactants enhances yield, lowers reaction temperature, and shortens reaction time by promoting micelle formation, thereby reducing organic solvent usage. The long-term objective is to incorporate eco-friendly methods in the synthesis process and to develop innovative oligomers with exceptional electronic properties.

References:

[1] M. Rooney, S. Mattiello, R. Stara, A. Sanzone, P. Brazzo, M. Sassi, L. Beverina, *Dyes and Pigments* **2018**, *149*, 893-901.

Donor-Acceptor-Substituted Squaraine Oligomers

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Building on an established synthetic strategy using protecting groups [1] we developed a method for the linear synthesis of energy donor-acceptor substituted squaraine oligomers. These donor-acceptor systems with up to four bridging squaraine units form a random coil or a helix superstructure depending on the solvent.[1] fs-Transient absorption spectroscopy prove ultrafast energy transfer from the energy donor to the acceptor on the order of several hundred femtoseconds. We are aiming to gain further insight into the energy transfer mechanisms between the respective moieties, by changing the oligo-squaraine bridge length, the type of the energy donor (perylene diimide vs. BODIPY), and the superstructure induced by the solvent.

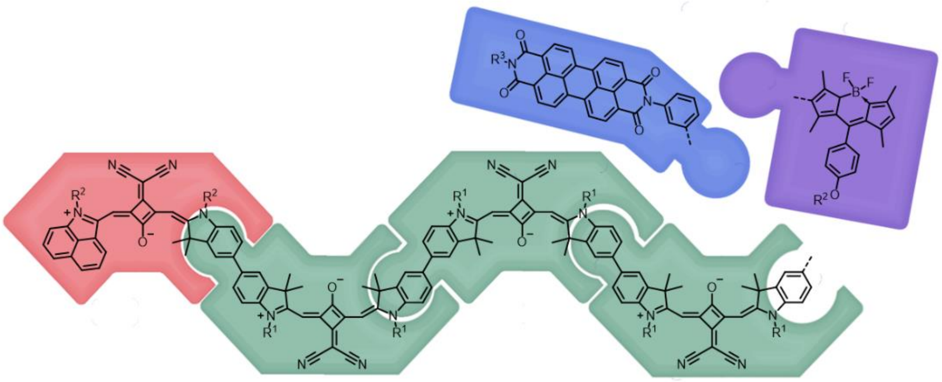

Figure 1: Heterosquaraine with acceptor (red), squaraine oligomer bridge (green) and different donor moieties, PDI (blue) and BODIPY (violet).

Referemces:

[1] Lambert *et al.*, *Chem. Eur. J.* **2021**, 27, 8380-8389.

Synthesis of porphyrin based supramolecular catalysts

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Homogeneous catalysis is an omnipresent topic in every field of chemistry. It provides new possible products, stabilizes reaction pathways and yields high stereo- and regio-selectivity. However, problems during catalysis can occur, making it necessary to search for new and alternative catalysts. Supramolecular catalysts mimic enzymes, which are nature's most potent catalysts, representing the gold standard of catalytically activity and selectivity.

Following the work of *Nitschke*[1] with his design and synthesis of a supramolecular cube and utilizing it as shown by *de Bruin*[2] on the field of supramolecular catalysis in order to enhance cyclopropanations, the assembly shown in figure 1 was build up from 3 building blocks. During the underlying work each step of the synthesis was checked for possible improvements and therefore, an adjusted procedure was found to form this supramolecular cage.

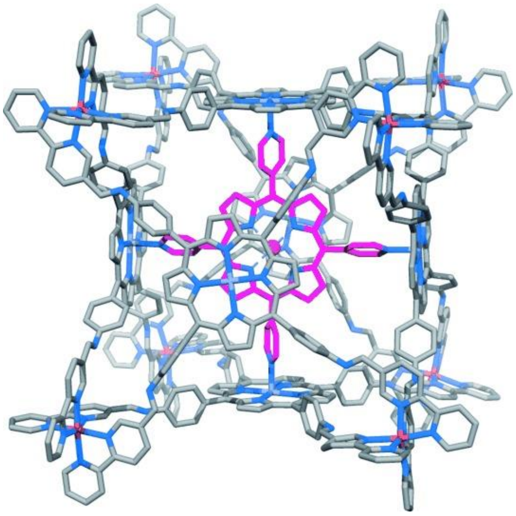

Figure 1: The figure shows a 3D-plot of the supramolecular catalyst, consisting of 6 times the same ligand, one on each face of the cubic system. Inside (pink) a cobalt-porphyrin is fixed, providing the catalytically activity of the assembly.

References:

[1] W. Meng, B. Breiner, K. Rissanen, J. D. Thoburn, J. K. Clegg, J. R. Nitschke, *Angew. Chem*. **2011**, *123*, 3541 –3545; *Angew. Chem. Int. Ed*. **2011**, *50*, 3479 –3483.

[2] M. Otte, P. F. Kuijpers, O. Troeppner, I. Ivanovic-Burmazovic, J. N. H. Reek, B. de Bruin, *Chem. Eur. J.* **2013**, *19*, 10170-10178.

Metallosupramolecular Cages from BINOL-Based Ligands

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BINOLs are versatile building blocks with various applications in asymmetric catalysis and are interesting in metallosupramolecular chemistry as C2 symmetric chiral building blocks due to their easy accessibility and modifications, most prominent in the 3 and 6 position directly accessible from BINOL. Other constitutional isomers can be synthesized by oxidative coupling of the naphthyl subunits. BINOLs display a high degree of rotational freedom along their 1,1'-axis which can also be limited through Williamson etherification to a specific angle between both naphthyl units by choosing a specific bridge. The coordinating motifs are easily introduced by cross-coupling reactions. So, a large family of related ligands with different size and geometry is easily accessible.

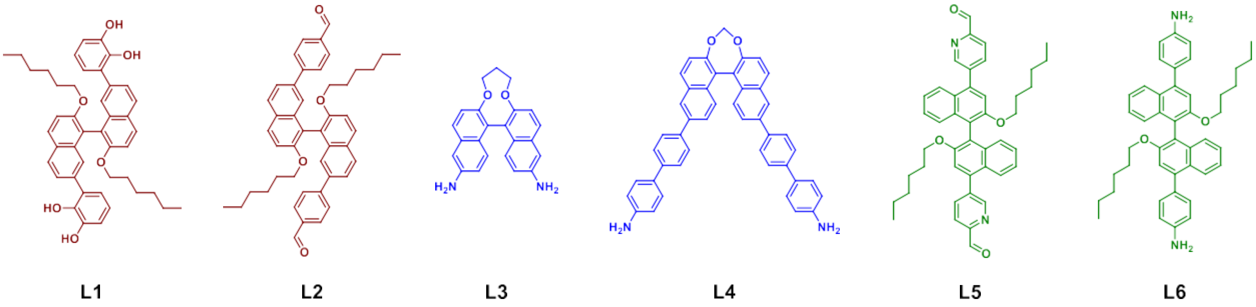

Figure 1: Overview of (pre)ligands for metallosupramolecular cages.

The subcomponent self-assembly approach in metallosupramolecular chemistry offers an easy synthesis of chelating ligands which can be used for aggregates based on the Symmetry Interaction approach. Octahedral iron(II) and cobalt(II) are employed for imine-based ligands and titanium(IV) for catechol-based ligands. Interchanging ligands and metal cations will have a significant impact on the formation, composition, geometry and properties of metallosupramolecular cages.

References:
[1] J. R. Nitschke, *Acc. Chem. Res.* **2007**, *40*, 103-112.
[2] N. Struch, C. Frömbgen, G. Schnakenburg, A. Lützen, *Eur. J. Org. Chem.* **2017**, *33*, 4984-4989.

Effect of Molecular Conformation on the Physical Properties of Three-dimensional Biradicaloids

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The marriage of a biradicaloid heptazethrene structure with helicenes leads to novel three-dimensional helically chiral biradicaloids, namely Helical Heptazethrenes (HHZ). This fusion results in a unique combination of physical properties of both classes of molecules. Our molecular design includes a straightforward synthesis, as well as an optimized strategy to separate the emerging stereoisomers. The outer edges of the helicene units of the enantiomers (*M**,*M**-HHZ) face in the same direction, while a continuous helical structure is formed in the *meso*-compound (*P,M*-HHZ). In this context, the effect of molecular conformation on the singlet–triplet energy gap, biradical character and chiroptical properties was investigated in particular.

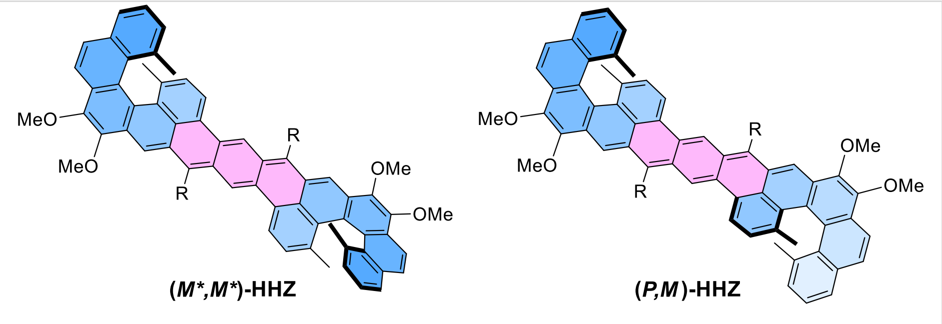

Figure 1: Emerging conformational diastereomers as result of the unique combination of biradicaloid heptazethrene and three-dimensional helicene structures.

References:

[1] P. Ravat, *et al.*, *Angew. Chem. Int. Ed.* **2016**, *55*, 1183-1186.
[2] Z. Sun *et al.*, *Angew. Chem. Int. Ed.* **2013**, *60*, 18229-18236.

Designing Organic π-Conjugated Molecules for Crystalline Solid Solutions: Adamantane-Substituted Naphthalenes

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We showcase herein organic crystalline solid solutions (CSSs)[1-3] based on the simplest polycyclic aromatic hydrocarbon (PAH) scaffold, naphthalene, stabilized by dispersion forces induced by adamantane substitution. High thermal stability of the host and guest molecules synthesized by cross-coupling of dibromonaphthalene derivatives and 4-(1-adamantyl)phenyl boronic ester enabled formation of crystals by sublimation. We could generate binary monocrystalline solid solution systems proven by X-ray crystallography, the first system of designed CSSs stabilized exclusively via dispersion forces with structural evidence. These observations are additionally supported by lattice energy calculations and spectroscopic examinations.[4]

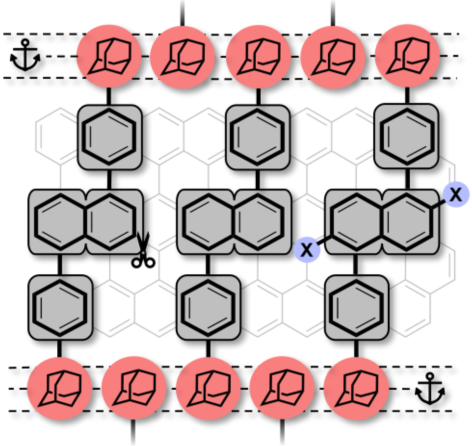

Figure 1: A schematic drawing of the design principle for PAHs with adamantane substituents.

References:

[1] M. Lusi, *Cryst. Growth Des*. **2018**, *18*, 3704–3712.
[2] A. I. Kitaigorodsky, *Mixed Crystals*, Springer Berlin, Heidelberg **1984**.
[3] F. Garelli, G. Ciamician, *Z. Phys. Chem.* **1896**, *21 U*, 113–126.
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Macrocyclic *meta*-Phenylene Bridged Dimers of Squaraine Dyes and their Self-Assembly in Solution

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Self-assembly phenomena give chemists the opportunity to build complex structures from small molecular units with possible new functionalities originating from the interactions of monomers within the aggregate.

In this work, a set of macrocyclic squaraine dimers **R-SQ₂** covalently bridged by *meta*-phenylene linkers carrying chiral substituents **R'** attached to the indolenine moieties were synthesised and characterised regarding their (chir)optical properties. The absorption spectra of the macrocycles show a pronounced hypsochromic shift (H-type) compared to those of the respective monomers. Self-assembly of the macrocycles in DMF or hexane to dimers is observed by concentration dependent absorption spectra. While the macrocycles are CD silent, their dimeric aggregates show pronounced CD signals suggesting a chiral twist-stacked aggregate structure.

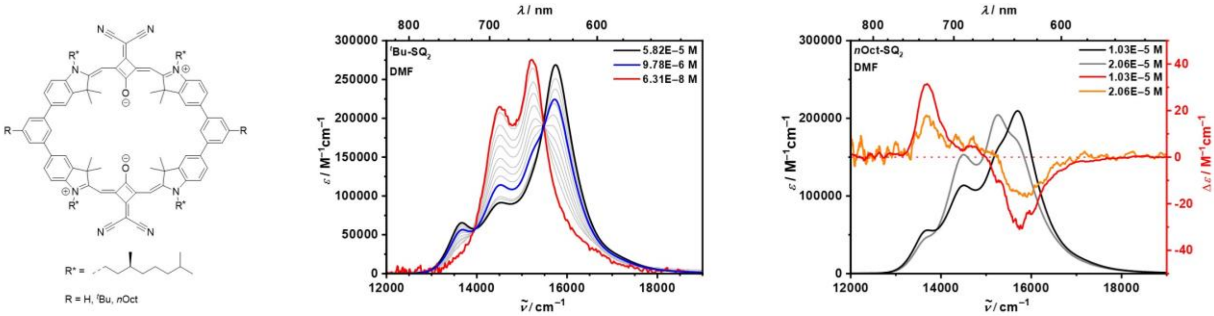

Figure 1: Left: Structure of **R-SQ$_2$**. Middle: Absorption spectra of **^{t}Bu-SQ$_2$** in DMF at different concentrations. Right: Concentration dependent absorption and ECD spectra of ***n*Oct-SQ$_2$** in DMF.

Semiconducting Starmesogens consisting of Subphthalocyanine Cores and Benzothienobenzothiophene/Oligothiophene Arms

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Subphthalocyanines (SubPc) **1** belong to a class of compounds intensely studied. This is owed to their application as non-fullerene acceptor for photovoltaic applications. [1] SubPc based liquid crystals can be aligned in the electric field and form highly polar columnar phases. [2] Such phases have been demonstrated to show the bulk photovoltaic effect.[3] This turns SubPc-based structures into attractive targets for materials science. Therefore, we became interested in umbrella-shaped SubPc star mesogens with oligothiophene arms (**2**). The strong SHG signal for these materials in the columnar phases can be explained by the generation of parallel dimers, in which the dipoles point along the columnar axis. [4] TOF mobility is in the range of $5 \cdot 10^{-3}$ cm^{2}V^{-1}s^{-1}. In the search for novel materials for organic electronics, we combine the SubPc core with benzothienobenzothiophene (BTBT) arms, as BTBT frameworks are among the best semiconductors known to date. [5]

Herein we present the challenging, successful synthesis of non-symmetric BTBT derivatives tailored for cross-coupling with the SubPC core via different linking units, resulting in target mesogens **3**-**5**. The impact of these units on thermotropic properties and the mesophase structure is studied by polarised optical microscopy (POM), differential scanning calorimetry (DSC) and X-ray scattering (XRS).

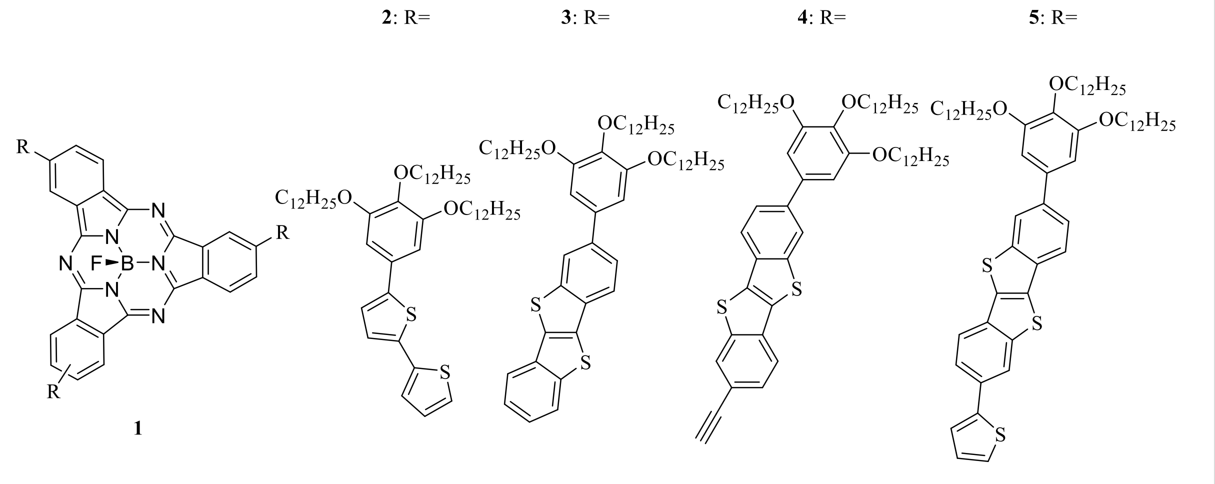

Figure 1: Structure of three different SubPC star mesogenes

[1] G. Lavarda, J. Labella, T. Torres; Chem. Soc. Rev., **2022**, 51, 9482.

[2] D. González-Rodríguez; T. Torres; *J. Mater. Chem. C*, **2015**, *3*, 985-989

[3] F. Araoka, *et al.*, *J. Am. Chem. Soc.* **2020**, *142*, 3326-3330.

[4] M. Lehmann, A. Eremin, M. Baumann, Adv. Funct. Mater., **2021**, *31*, 2104217

[5] Y. H. Geerts *et al.*, *J. Org. Chem.* 2013, 78, 15, 7741-7748

Nanoscale π-conjugated ladder oligomers and polymers

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Ladder polymers are defined by the IUPAC as polymers “which consist of an uninterrupted sequence of rings with adjacent rings […] having two or more atoms in common”.[1] Herein we report on *π*-conjugated rails that are connected repeatedly by stiff rungs to create a well-defined and rigid ladder oligomers and polymers. The synthesis focuses on two ladder polymers: A donor-acceptor ladder polymer and a three stranded ladder polymer. The synthesis begins with the construction of monomers from four building blocks. The synthesis is characterized by *Sonogashira* couplings. Ladder monomers can be polymerized according to the zipping strategy, whereby a single-stranded polymer precursor is polymerized first. Afterward, an intramolecular zipping reaction closes the open prepolymer.

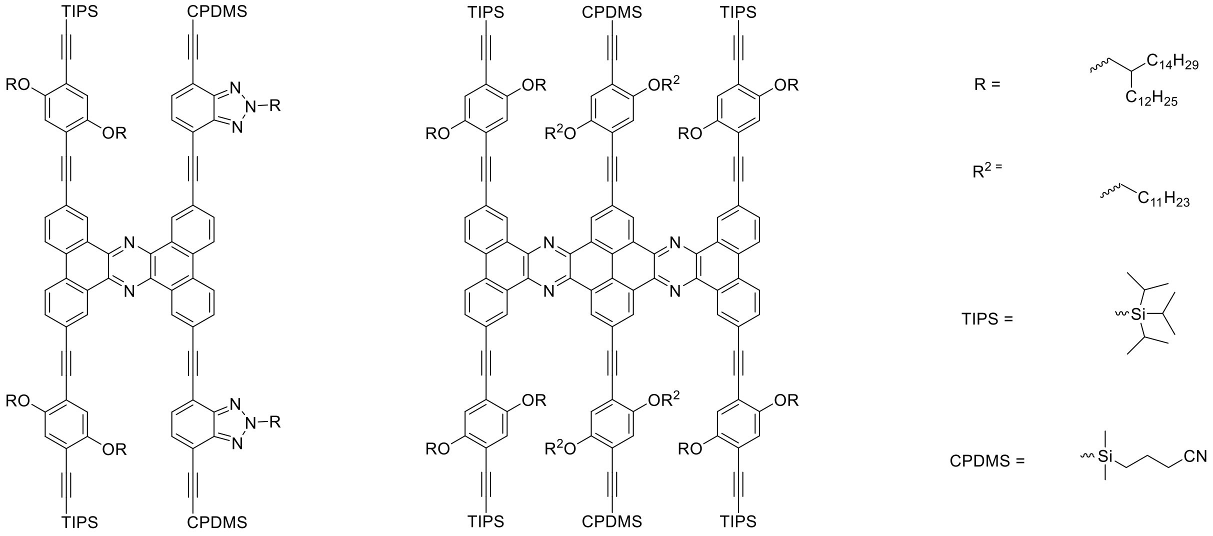

Figure 4: Left: donor-acceptor monomer; Right: three-stranded monomer.

References:

[1] W. V. Metanomski, R. E. Bareiss, J. Kahovec, K. L. Loening, L. Shi, V. P. Shibaev, *Pure Appl. Chem.* **1993**, *65*, 1561
[2] S. Meißner, J. M. Lupton, S. Höger, *et al.*, *Nat. Commun.* **2021**, *12*, 6614.
[3] T. Eder, J. Vogelsang, S. Bange, K. Remmerssen, D. Schmitz, S.-S. Jester, T. J. Keller, S. Höger, J. M. Lupton, *Angew. Chem. Int. Ed.* **2019**, 58, 18898–18902.

Exo-BODIPY, *Endo*-Alkoxy Functionalized Pd_2L_4 Cages

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Self-assembled coordination cages (SCCs) show favorable properties for an array of applications like drug delivery, host-guest chemistry, and catalysis. Modification of the SCCs interiors by installation of *endo* facing functionalities on the constituent ligands gives control over properties like guest binding, catalytic activity, or inducement of self-sorting effects.[1] Additionally, SCCs have received increasing attention for light harvesting applications, as their reliable self-assembly is predestined to arrange multiple chromophoric units in a fixed spatial arrangement, thus facilitating control over the rates of energy transfer. [2]

In this study we present the synthesis of a series of *endo*-alkoxy, *exo*-BODIPY functionalized 1,3-bis(3-pyridyl) ligands and their self-assembly into Pd_2L_4 coordination cages (Figure 1). All these cages show intense fluorescence which may be harnessed for light harvesting applications. Additionally, these complexes show distinct changes in their ^{1}H-NMR spectra, dependent on the length of the *endo* facing alkoxy groups, thus highlighting the impact such modifications may have on the self-assembly of SCCs.

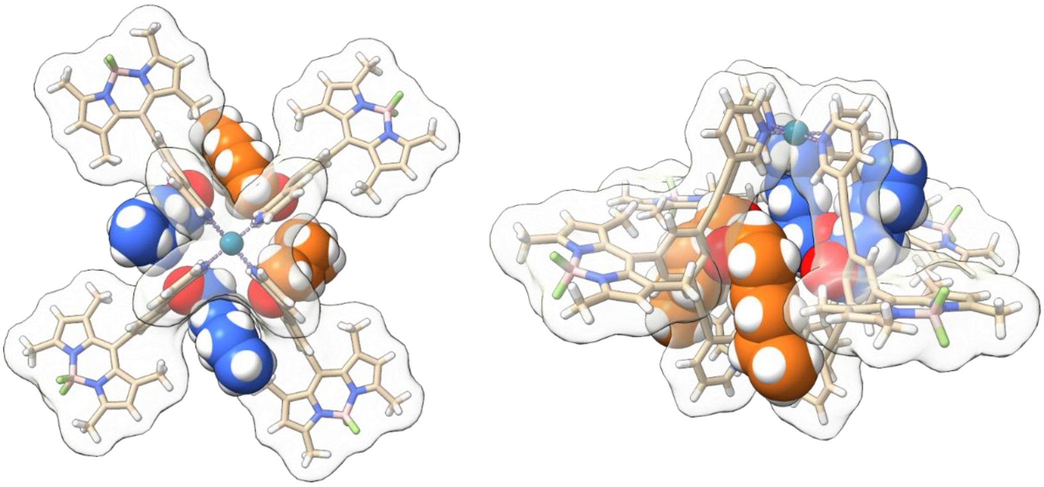

Figure 1: Crystal Structure of a self-assembled Pd_2L_4 cage. The *endo* directed hexadecyloxy-chains are closely packed between the backbones of two neighboring ligands and point either up or down (marked in blue and orange, respectively).

References:

[1] P.M. Bogie, T.F. Miller, R.J. Hooley, *Isr. J. Chem.* **2019**, 59, 130-139.
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New fluorescent dimers in DNA

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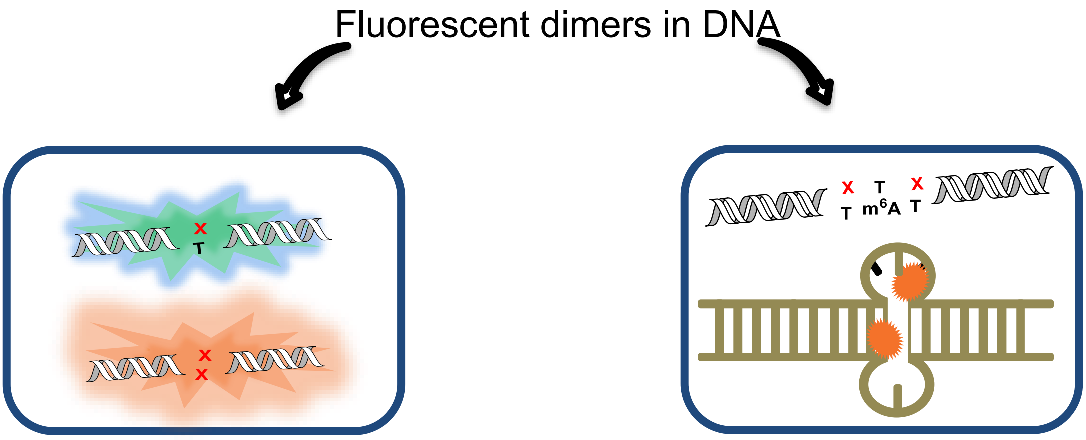

Figure 1: DNA duplex with monomer and dimer (**left**), DNA probe to detect m^{6}A modification (**right**).

DNA contains the blueprint for the entire organism. A mutation of one base, a so-called single nucleotide polymorphism (SNP), can have considerable consequences. One possibility to detect such changes in DNA are fluorogenic probes, which sensitively reveal the SNPs by a wavelength shift of the fluorescence. The aim of this work is the formation of new fluorescent dimers in DNA, which shows a bathochromic shifted fluorescence compared to the monomer. On the one hand, dimers are to be generated in the double strand, in which one dye is present per strand, and on the other hand, dimers are to be generated in the double strand, in which both dyes are present in the same single strand. This dimer formation will be used to synthesize a DNA probe that detects an N^6-Methyladenosine (m^{6}A) modification by hybridization.

References:

[1] DIDENKO, Vladimir V. DNA probes using fluorescence resonance energy transfer (FRET): designs and applications. Biotechniques, 2001, 31. Jg., Nr. 5, S. 1106-1121.

[2] Berndl, S. (2010). Fluoreszente H-Aggregate von Thiazol Orange in DNA und RNA, sowie postsynthetische Klick-Ligation an DNA (Doctoral dissertation, Universität Regensburg).

Synthesis and On-Surface Preparation of Pentadecacene

Non-Covalent Approach to harvest delayed fluorescence and phosphorescence in Naphthalene Bisimide Cyclophane

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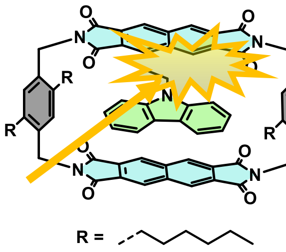
Organic light emitting diodes (OLEDs) recently received immense attention in the scientific community due to their ability to utilize 100 % exciton theoretically. However, the efficiency of traditional OLED devices is limited to 25 % due to the major loss of 75 % of non-emissive triplet states at room temperature.[1] In 2012, Adachi's group revitalized the application of Thermally Activated Delayed Fluorescence (TADF) materials, which demonstrated that TADF is an efficient process to harvest non-emissive triplet-state to enhance the internal quantum efficiency (IQE) of OLED devices.[2] The typical TADF molecules usually involve twisted covalently attached donor-acceptor (D-A) architecture with near orthogonality to decrease the electronic exchange energy (*J*). However, the supramolecular approach for TADF design can endow TADF emission in the solution state. Herein, utilizing the well-known building block of arylene bisimide, we show the potential of supramolecular strategy to achieve TADF emission in air. The figure below shows the unique character of air-stable triplet states, demonstrating TADF behavior by a non-covalent approach achieved using cyclophane molecular design.



delayed fluorescence lifetime (in air): 0.4 – 1.6 μs; photoluminescence quantum yield (in air): 5-7 %

Figure 1: Molecular design of supramolecular system to harvest air-stable triplet states by TADF approach.

References:

[1] Y. Zhang, S. R. Forrest, *Physical Review Letters* **2012**, *108*, 26-29.
[2] H. Uoyama, K. Goushi, K. Shizu, H. Nomura, C. Adachi, *Nature* **2012**, *492*, 234–238.

A Novel Symmetric Chiral Squaraine – A New Starting Point

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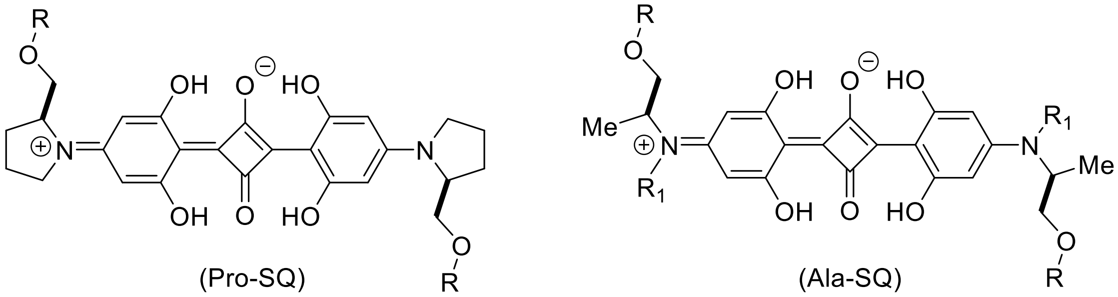
Both chiral squaraines and the achiral representative of this molecule class are fascinating and intriguing compounds for optoelectronic devices.[1-4] Especially the chiral squaraines are of utmost interest due to translation of the inherent chirality from the molecular level onto the supramolecular level, as observed in an impressive circular dichroism.[1,3] This was observed in the well-investigated proline-derived anilino squaraines (Pro-SQ) (Figure 1).



(Pro-SQ)
proline-derived anilino squaraines

(Ala-SQ)
alaninol-derived anilino squaraines

Figure 1: left: general structure of Pro-SQs with varying alkyl-residues; right: general structure of Ala-SQs with varying alkyl-residues (R, R^1= alkyl chains).

In order to expand the existing substance library of chiral sqauraines and following the ex chiral pool approach, as previously shown in the case of Pro-SQs, an amino acid was chosen as the starting material, in this case L-alanine or its reduced form L-alaninol respectively. This gives rise to the new class of squaraines: the alaninol-derived anilino squaraines (Ala-SQ). The first representative of this class is *N*-Butyl, *O*-Butyl-Ala-SQ.

References:

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Investigation of BN doped PAHs based on a Paracyclophane scaffold

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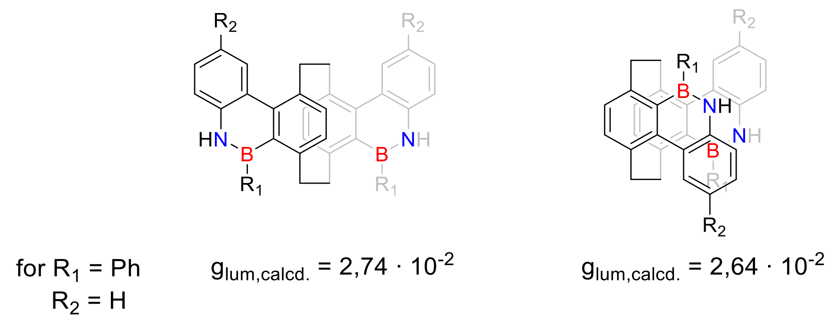
Boron–nitrogen-doped π-conjugated systems often possess exceptional electronic and optical properties, which qualifies their chiral representatives as promising emitters of circularly polarized light (CPL).[1] In previous studies, our group already demonstrated that the attachment of BN doped fluorophores to chiral scaffolds enables synthesis of potent CPL emitters.[2]



for R_1 = Ph
R_2 = H

$g_{lum,calcd.} = 2{,}74 \cdot 10^{-2}$

$g_{lum,calcd.} = 2{,}64 \cdot 10^{-2}$

Figure 1: Target Molecules along with the computed dissymmetry factors (g_{lum}) at the TD-M06-2X/def2-TZVP level of theory.

One of our current research projects focuses on the extension and BN-doping of the π- system of [2.2]Paracyclophane. The target molecules (Figure 1) were identified as potent CPL emitters in preliminary computational studies. The synthesis route of these compounds is currently under investigation.

References:

[1] X. Chen, D. Tan, D. Yang, *J. Mater. Chem. C,* **2022***,* 10, 13499-13532.
[2] M. Rapp *et al*., *J. Mater. Chem. C,* **2023**, 11, 15767-15773.

Magnetic High Field Effects in Chalcogen Substituted Donor-Acceptor Dyads

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Charge separated states of donor-acceptor compounds can be considered as spin-correlated radical pairs whose lifetimes can be influenced by an external magnetic field. By substitution of the 1,7 positions of a perylene diimide acceptor in a donor-acceptor dyad **X-Dyad** with chalcogen substituents (X = OPh, SPh, SePh, TePh), we observed a pronounced high field effect in the decay of the charge separated state by using magnetic field dependent ns-transient absorption spectroscopy. This can be explained by a *g*-tensor anisotropy induced spin relaxation, leading to an increased S-T mixing at high magnetic fields, particularly for the selenium derivative.

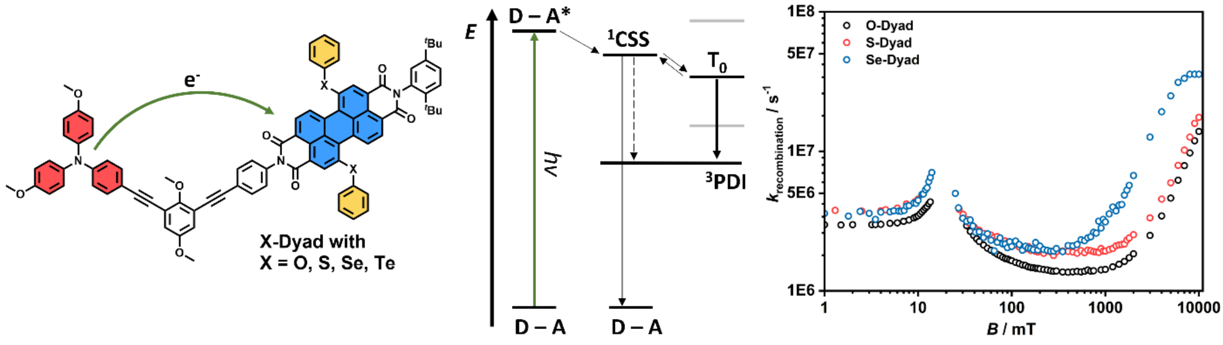

Figure 1: Left: X-Dyads for the investigation of magnetic field effect. Middle: State diagram Right: Observed recombination rates for the X-Dyads.

References:

[1] P. Mentzel, M. Holzapfel, A. Schmiedel, I. Krummenacher, H. Braunschweig, A. Wodynski, M. Kaupp, F. Würthner, C. Lambert, *Phys. Chem. Chem. Phys.*, **2022**, *24*, 26254-26268.

Synthesis and On-Surface Preparation of Pentadecacene

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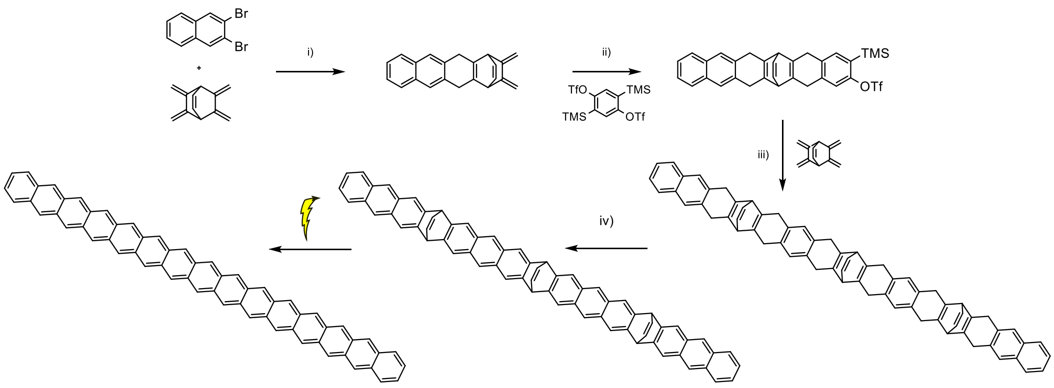
With increasing number of rings, the HOMO-LUMO gap of the acenes decreases while the (poly)radical character increases. For the comprehensive understanding of the fundamental properties of acenes their expansion towards even longer homologues is necessary. Tridecacene has been prepared recently via STM tip-induced conformational preparation and dissociation of triethenobridged precursors on a Au(111) surface.[1] We here report the synthesis of a pentadecacene precursor.



i) n-BuLi, toluene, -60 °C, 3 h; ii) MeCN, CsF, 45 °C, 19 h; iii) DCM, MeCN, KF, 18-crown-6, RT, 16 h; iv) DDQ, $CHCl_3$, RT, 2 h; v) Au(111), STM tip, 4 K

Figure 1: Generation of the pentadecacene.

References:

[1] Z. Ruan, J. Schramm, J. B. Bauer, T. Naumann, H. F. Bettinger, R. Tonner-Zech, J. M. Gottfried, *J. Am. Chem. Soc.* **2024**, *146*, 3700.
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BN-Doped Fluorophores as Fluorescent Uridine Analogues

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Fluorescent nucleobases are novel tools used in a wide variety of chemical, biophysical, structural, and biomedical applications. Polycyclic aromatic hydrocarbons (PAHs), like pyrene, phenanthrene or perylene have been used either as non-canonical nucleobases or linked to common canonical nucleobases, to combine the advantages of an extended fluorophore and the ability for base pairing.[1] BN-doping of such fluorophores results in tuned photophysical properties.[2] We prepared unprecedented organic–inorganic hybrid nucleosides, by synthesizing ethynyl substituted BN-doped phenanthrene and pyrene compounds and coupled them with 5-iodo-2'-deoxyuridine.[3] The novel nucleosides showed different stability properties and photophysical behaviors.

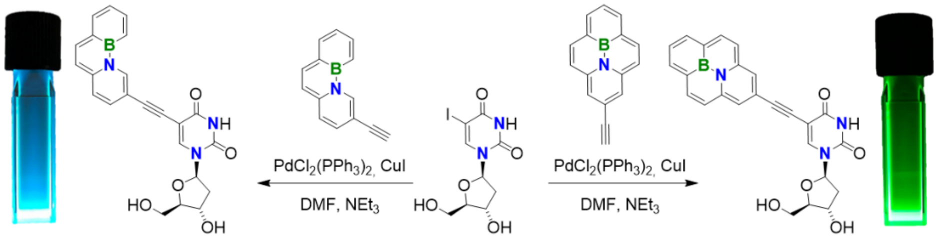

Figure 1: Synthesis of the BN-nucleosides and fluorescence thereof under UV irradiation.

References:

[1] a) W. Xu, K. M. Chan, E. T. Kool, *Nat. Chem.* **2017**, *9*, 1043-1055; b) C. Steinmetzger, C. Bauerlein, C. Höbartner, *Angew. Chem. Int. Ed.* **2020**, *59*, 6760-6764.

[2] a) J. D. Bosdet, C. A. Jaska, W. E. Piers, T. S. Sorensen, M. Parvez, *Org. Lett.* **2007**, *9*, 1395-1398; b) J. D. Bosdet, W. E. Piers, T. S. Sorensen, M. Parvez, *Angew. Chem. Int. Ed.* **2007**, *46*, 4940-4943.

[3] M. Müller, H. Neitz, C. Höbartner, H. Helten, *Org. Lett.* **2024**, *26*, 1051-1055.

[7]Helicene-based Pd_3L_6 coordination cage

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The class of helicenes has constantly attracted interest in the chemical community due to their fascinating structure. Initially only a chemical curiosity, the focus has been shifted towards physico-chemical properties and applications. Among others, the rigid structure paired with their helical chirality has been exploited in stereoselective synthesis, supramolecular aggregates and optoelectronics.[1]

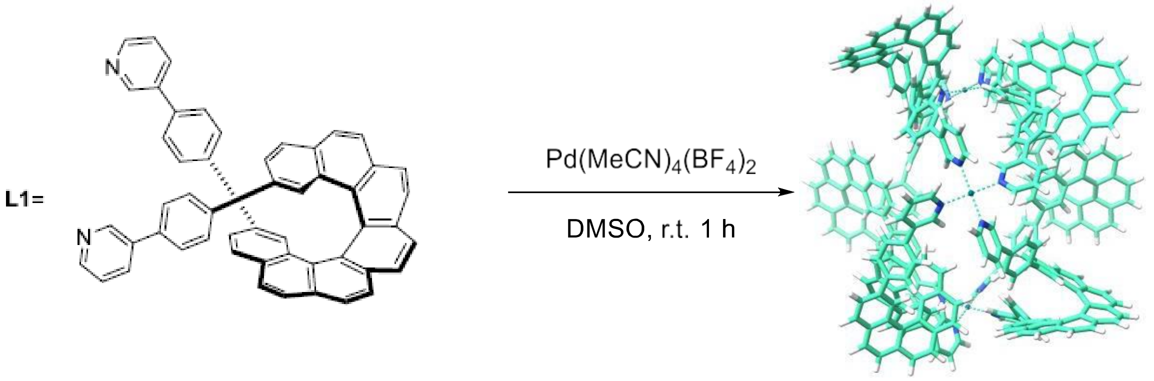

Figure 1: Pd_3L_6 frmation from [7]helicene-based bispyridyl ligand L1 and Pd(II) ions.

Herein, we report a helicene-based Pd_3L_6 coordination cage. A racemic mixture of the bis-pyridyl ligand with a [7]helicene backbone assembles with square planar Pd(II) cations to a complex mixture of different Pd_3L_6 cages. Generally, a complex consisting of three Pd(II) centers and six bis-monodentate ligands can adopt up to seven different topologies, four of them being chiral.[2] Upon resolving the enantiomers of L1 by HPLC, the enantiopure ligands were observed to not only assemble into the cage with the highest symmetry, but likely into all seven possible cages.

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Peri-Functionalized Tetraazaperylenes: A New Class of Strong Emitters

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The interest in the chemistry surrounding polycyclic aromatic compounds has experienced a revival as the result of the use of functional dyes as electronic materials, primarily due to the tunability of their photophysical and redox properties.[1] Among the plethora of published compounds, tetraazaperylene derivatives have distinguished themselves from other highly emissive and redox active functional dyes, because of their capability of having their peri and bay positions independently modified via nucleophilic substitutions and/or metal catalyzed coupling reactions.[1] This has led to the development of fluorophore systems such as octaazaperopyerene (OAPPs),[2] and octaazaperopyrenedioxides (OAPPDOs),[3] in both cases limited structural variability has had a significant impact on the electronic structures of these compounds.[2,3]

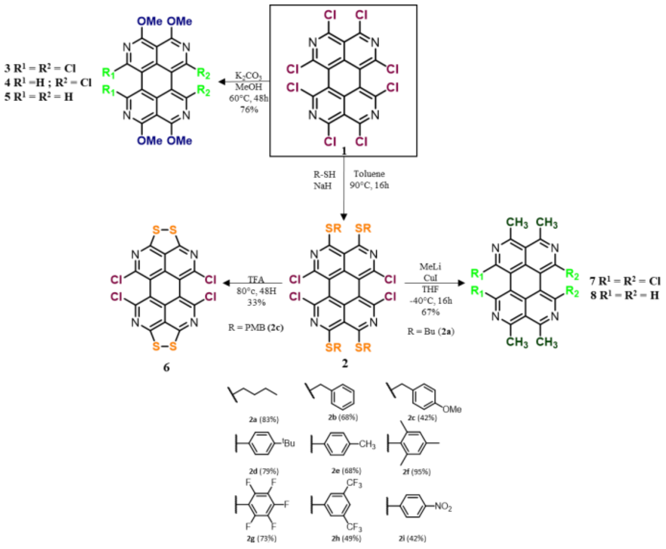

Figure 1. Derivatives of octaclorotetraazaperylene References

(1) T. Wesp, P. Valsalan, A. Kochan, M. Hertzog, H. Wadepohl, J. Zaumseil, L. H. Gade, *Chem. Eur. J.*, **2022**, *28*, e202202661.

(2) T. Wesp, T. Bruckhoff, J. Petry, H. Wadepohl, L. H. Gade, *Chem. Eur. J.* **2022**, *28*, e202200129.

(3) T. Wesp, T. Bruckhoff, H. Wadepohl, L. H. Gade, *Chem. Eur. J.* **2022**, *28*, e202201706.

Sequence specific synthesis of DNA-chromophore architectures as light harvesting systems

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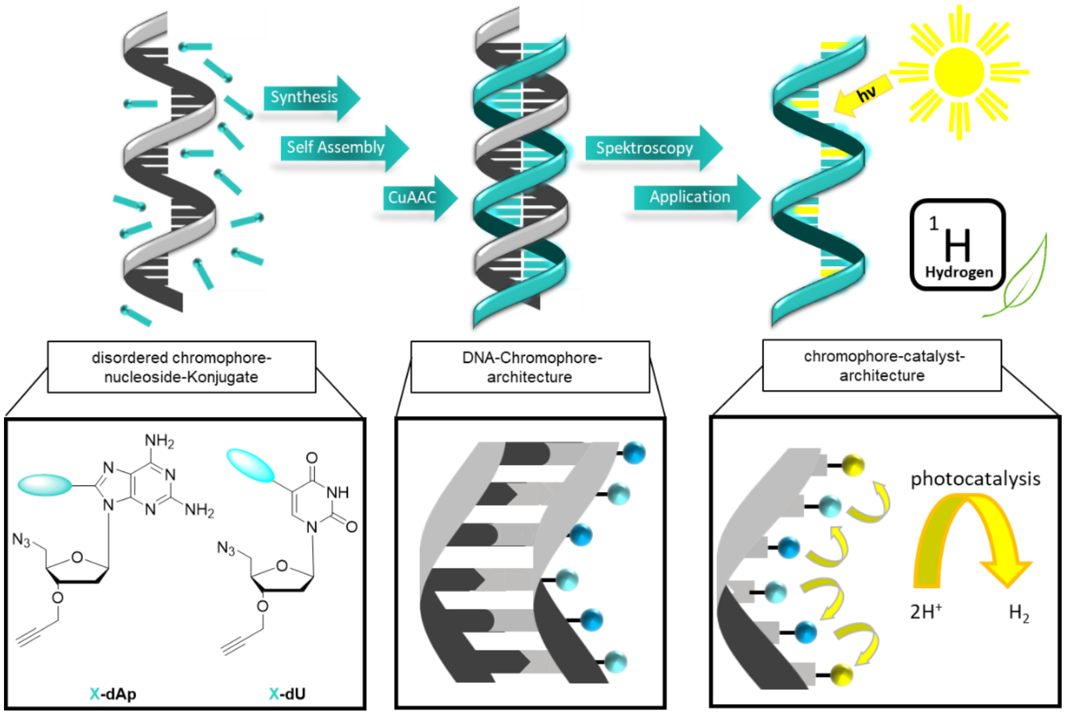

Figure 5: Sequence-specific assembly of disordered chromophore nucleoside conjugates (left) to defined DNA chromophore architectures (center) and the planned use as a light harvesting system (right).

Organic light harvesting systems will play an important role in securing the global demand for renewable energy. The aim is to make full use of the solar spectrum possible and to provide access to green hydrogen in conjunction with suitable photocatalysts.

Due to the canonical base pairing, DNA offers itself as a structure-giving template to ensure a precise arrangement of the chromophores and thus a cost-effective generation of such functional structures. A fixation of the chromophores in the self-assembled sequence via a biocompatible triazole backbone has not yet been realized. This is the next and decisive step towards new, stable light harvesting systems.

References:

[1] N. Armaroli, V. Balzani, *Angew. Chem. Int. Ed.* **2007**, *46*, 52-66.
[2] P. Ensslen, H.A Wagenknecht, *Chem. Eur. J.* **2015**, *21*, 9349-9354.
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New *π*-conjugated nanoscale ladder polymers

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A fascinating class of polymers deals with *π*-conjugated ladder polymers (cLPs), which consist of an uninterrupted sequence of adjacent rings sharing at least two atoms. Therefore, the polymer does not break apart if one of the two strands breaks and cLPs are thus expected to possess a high resistance to thermal, mechanical and chemical degradation. [1] Furthermore, most cLPs own an exceptionally rigid structure, in which the two strands are held at a discrete distance defined by the spacer. This allows investigation of the influence of interchain interactions (H-type coupling) between the two *π*-conjugated strands as well as intrachain interactions (J-type coupling) within the strands and HJ-type aggregate formation by means of single molecule fluorescence spectroscopy.[2]

A fully *π*-conjugated, pyrene-based monomer was synthesized. The monomer was oligomerized according to the "zipping strategy" in a sequence of an acetylene-deprotection followed by an oligomerization under *Glaser-Eglinton* conditions and separation of the oligomers performed by gel permeation chromatography. The dimer and tetramer LP were obtained after deprotection using TBAF and closure of the second strand under *Glaser-Eglinton* conditions.

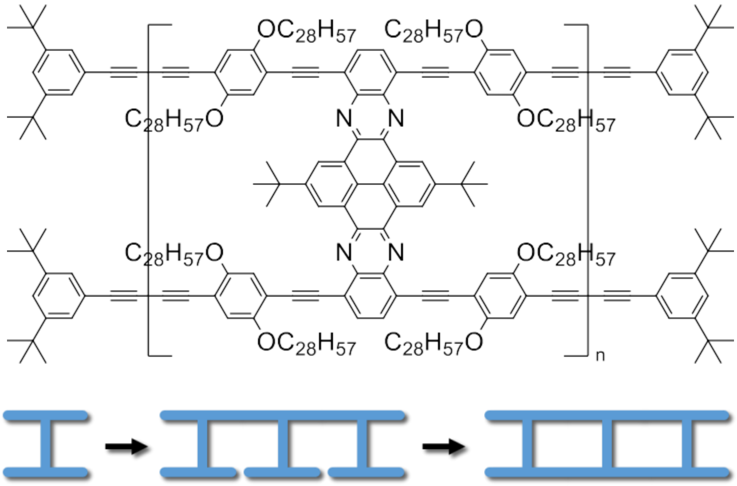

Figure 1: a) shows the structure of a new pyrene-based, fully *π*-conjugated ladder oligomer and b) a schematic illustration of the oligomerization strategy.

References:

[1] a) W. V. Metanomski, R. E. Bareiss, J. Kahovec, K. L. Loening, L. Shi, V. P. Shibaev, *Pure & Appl. Chem.* **1993**, *65*, 1561; b) A.-D. Schlüter, *Adv. Mater.* **1991**, *3*, 282.

[2] C. Allolio, T. Stangl, T. Eder, D. Schmitz, J. Vogelsang, S. Höger, D. Horinek, J. M. Lupton, *J. Phys. Chem. B* **2018**, *122*, 6431.

Dimerization and Rearrangement of Fluorene Based Dialkynes

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Circumazulene is a polycyclic aromatic hydrocarbon, consisting of an upper half with a five-membered ring and a lower half with a seven membered ring.[1] During our attempted synthesis of the upper half, we serendipitously discovered a rearrangement reaction of fluorene based dialkynes as well as an expanded scope for their dimerization.[2] To study electronic effects on these competing reactions, several substituents were introduced. To further elucidate the underlying reaction mechanism of the rearrangement, pathways leading to the benzannulation and rearrangement were calculated by DFT-methods. Both the rearranged and dimerization products were studied for their optoelectronic properties.[3]

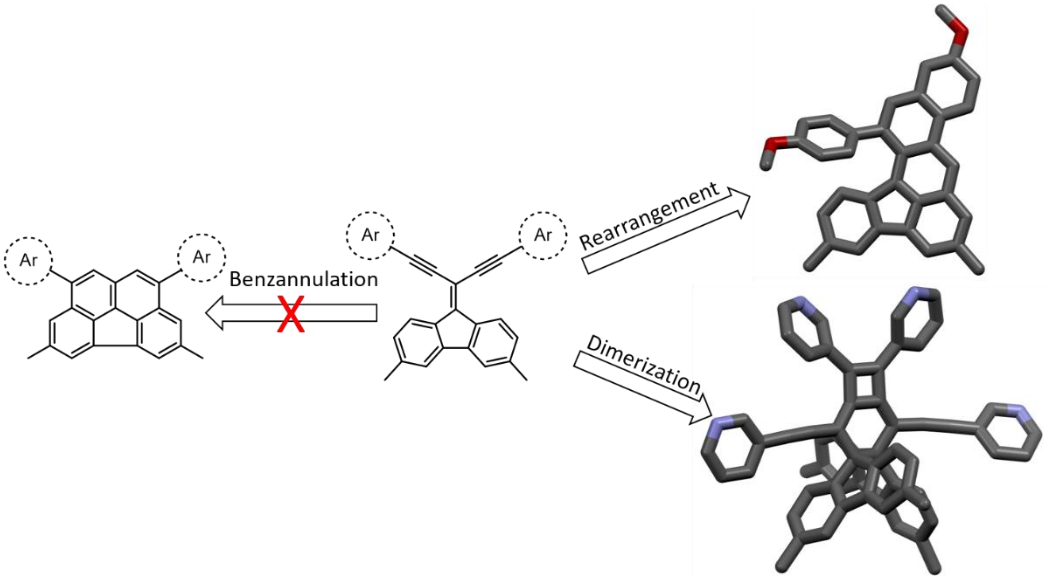

Figure 1: Fluorene based dialkynes and their reactivity under platinum catalyzed benzannulation conditions.

References:

[1] F. Wu *et al.*, *Chemistry* **2023**, *29*, e202301739.
[2] H. Hopf *et al.*, *Angew. Chem. Int. Ed. Engl.* **2003**, *36*, 1187-1190.
[3] Our work*, manuscript in preparation.*

New Non-Fullerene Acceptor-based Materials for Circularly Polarized Light Detection

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Photodetectors that can convert circularly polarized light into electrical signals, have different applications in satellite communication, 5G technologies, and more advanced sensing technologies. One way to achieve circularly polarized light detection is to use materials which can directly discriminate between left- and right-handed circularly polarized light.[1] A promising material class for this application are Non-Fullerene Acceptors (NFAs) which are typically used as acceptor materials in organic photovoltaics. As *Wan et al*.[2] and *Liu et al*.[3] have shown, these NFAs can be used in circularly polarized light detectors by mixing them with a chiral inducer (g_{abs} = 0.15)[2] or by introducing chiral alkyl side chains (g_{abs} = 0.04).[3]

In this work, the interactions between the chiral inducer and the NFA are further investigated, and new chiral materials are synthesized to optimize the chiroptical properties and the device performance of circularly polarized light detectors. A simple chiral NFA was already synthesized which shows a promising absorption dissymmetry factor of up to g_{abs} = 0.24 as a pristine thin film on glass and promising performance with **PBDB-T** in BHJ-photodiodes.

References:

[1] M. Schulz et al., *Adv. Funct. Mater.* **2019**, 29, 1900684.
[2] L. Wan et al., *Nat. Photon.* **2023**, 17, 649–655.
[3] L. Liu et al., *Small* **2022**, 18, 2202941.

Synthesis and Investigation of a chiral Nanodoublehoop

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In recent years, cycloparaphenylenes (CPPs) and their derivatives have attracted significant attention due to their diverse optical and supramolecuar properties and potential applications.[1] Dibenzo[*a,e*]pentalenes (DBPs) exhibit a narrow HOMO-LUMO gap and demonstrate ambipolar electrochemical behavior, making them particularly attractive for organic devices.[2] Consequently, combining CPPs with DBP provides further insights into the structure-property-relationship behavior of bent antiaromatics.[4]

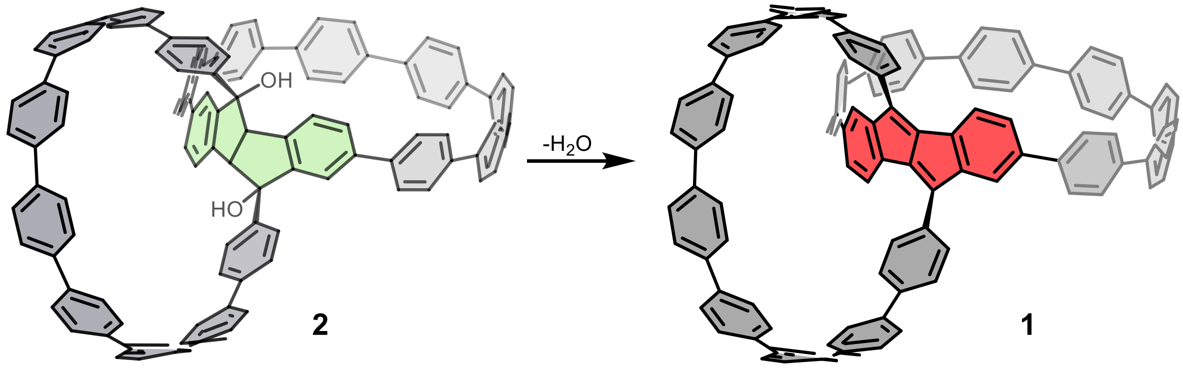

Figure 1: Synthesis of DBP based double hoop from fluorescent precursor.

We herein present the synthesis of a novel chiral double-hoop **1** along with its fluorescent precursor **2**. The connection of the CPP parts via both the 5- and 6-membered rings is established. Sequential ring strain introduction facilitated the incorporation of the CPP segments. Additionally, enantiomeric separation of the fluorescent diol precursor was achieved, followed by the measurement of circular dichroism and circularly polarized luminescence spectra. This analysis offers valuable insights into the chiroptical properties and optoelectronic behavior of chiral double-hoops.

References:

[1] E. J. Leonhardt, R. Jasti, *Nat. Rev. Chem.* **2019**, *3*, 672–686.
[2] M. Hermann, R. Wu, D. C. Grenz, D. Kratzert, H. Li, B. Esser, *J. Mater. Chem. C* **2018**, *6*, 5420–5426.
[3] P. Seitz, M. Bhosale, L. Rzesny, A. Uhlmann, J. S. Wössner, R. Wessling, B. Esser, *Angew. Chem. - Int. Ed.* **2023**, *62*, e202306184

Contribution to the synthesis of Organic Electro-optic Materials

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Electro-optic modulators play a key factor in the rapid conversion of signals in the electric to the optical domain, allowing nearly light-speed communication.[1] Classic modulators, made from silicon, fail to reach a modulation of more than 100 GHz. In contrast, organic based electro-optic materials utilizing π-electron systems could theoretically achieve bandwidths in the terahertz region.[2] This work aims to design nonlinear optical chromophores with a central TIPS-anthracene building block in the form of a D-π-A system using DFT calculations and synthesize them using common methods.

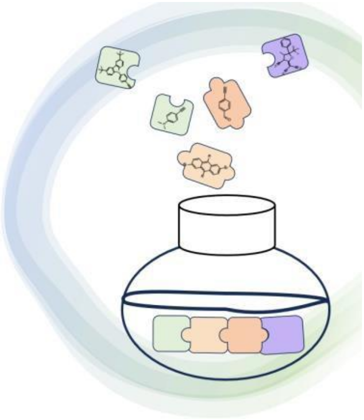

Figure 1: Selection of potential D-π-A system building blocks. The different building blocks are picked according to their performance in computational calculations in various combinations of target molecules.

References:

[1] G. Sinatkas, T. Christopoulos, O. Tsilipakos, E. E. Kriezis, *J. Appl. Phys.* **2021**, *130*
[2] M. Lee, H. E. Katz, C. Erben, D. M. Gill, P. Gopalan, J. D. Heber, D. J. McGee, *Science* **2002**, *298*, 1401–1403.

Donor-Acceptor Complex Formation by Social Self-sorting of Polycyclic Aromatic Hydrocarbons and Perylene Bisimides

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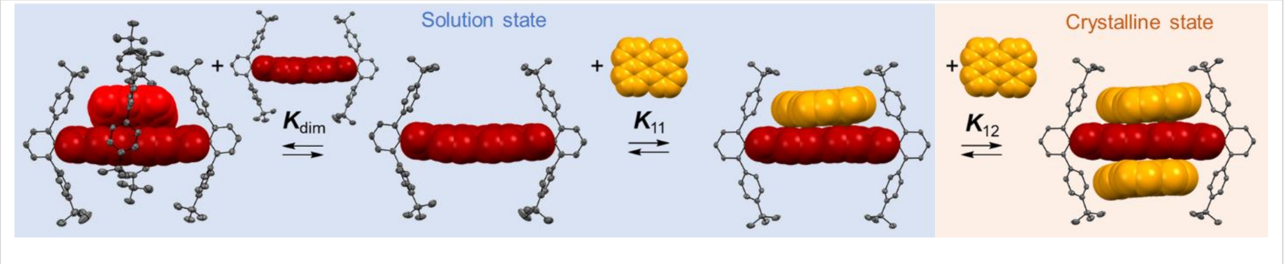

Figure 1: Perylene bisimides equipped with bulky imide substituents self-assemble into orthogonally stacked dimers or bind up to two polycyclic aromatic hydrocarbons.

Electron-donor–acceptor (EDA) complexes between electron-rich and electron-poor π-scaffolds are desired in the solid state for various applications[1] and even more in solution for fundamental photophysical studies.[2] However, EDA complexes between the electron-poor perylene bisimides (PBIs) and electron-rich polycyclic aromatic hydrocarbons (PAHs) could so far only be realized in solution with PBI cyclophane supramolecular hosts.[3]

Here, self-assembly versus complexation with PAH guest molecules is studied for a series of PBIs in solution as well as in the solid state. Bulky imide substituents at the chromophore guide their self-assembly into discrete dimer aggregates with null-type exciton coupling. Host-guest titration experiments with different PAHs afford 1:1 and 1:2 complexes whose properties are studied by single crystal X-ray analysis as well as UV/Vis and fluorescence spectroscopy.[4]

References:

[1] D. S. Weiss, M. Abkowitz, *Chem. Rev.* **2010**, *110*, 479-526.
[2] P. Spenst, R. M. Young, M. R. Wasielewski, F. Würthner, *Chem. Sci.* **2016**, *7*, 5428-5434.
[3] P. Spenst, F. Würthner, *Angew. Chem. Int. Ed.* **2015**, *54*, 10165–10168.
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Synthesis of porphyrin-based supramolecular catalysts

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The encapsulation of transition metal catalysts into the cavity of a self-assembled supramolecular aggregate leads to the formation of a supramolecular flask. This approach is inspired by the function of nature's enzymes. The shielding of the catalyst within the cavity increases its lifetime and allows control of the second coordination sphere of the catalytic transition metal, which can influence substrate and product selectivity.[1-3]

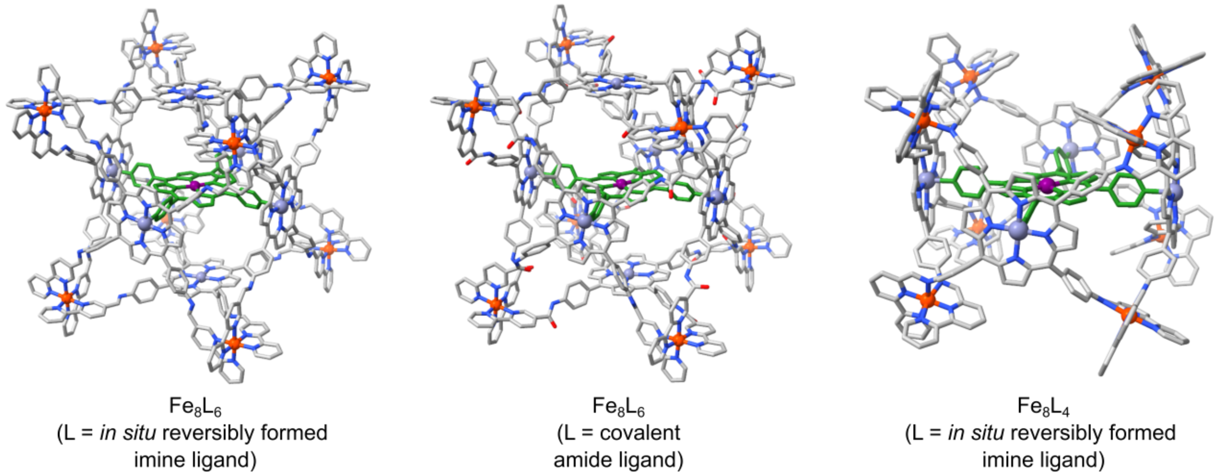

Figure 1: MMFF-minimized model structures of synthesized and envisioned supramolecular catalysts.

The aim is the synthesis of multiple porphyrin-based supramolecular catalysts with different structural properties. In the future, by performing catalytic reactions within these cavities, the influence of differently shaped microenvironments on the selectivity and performance of the encapsulated transition metal porphyrin can be compared.

References:

[1] S. H. A. M. Leenders, R. Gramage-Doria, B. de Bruin, J. N. H. Reek, Chem. Soc. Rev. **2015**, *44*, 433–448.
[2] M. Yoshizawa, J. K. Klosterman, M. Fujita, *Angew. Chem. Int. Ed.* **2009**, *48*, 3418–3438.
[3] T. S. Koblenz, J. Wassenaar, J. N. H. Reek, *Chem. Soc. Rev.* **2008**, *37*, 247–262.

Statistical Self-Assembly of Catalytically Active Heteroleptic Metallosupramolecular Cages

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The concept of catalytically active metallosupramolecular cages is inspired by nature's enzymes and mimics their confined microenvironments that allow selective chemical transformations.[1] The envisioned discrete heteroleptic M_2L_4 or $M_{12}L_{24}$ cages consist of concave bis(pyridyl) ligands and Pd(II) or Pt(II) cations. In a statistical approach, NCN-Pt-azide *endo*-functionalized analogues of the ligands will be incorporated into the cages. Post-assembly, the catalytically active species is obtained *via* photochemically induced N_2 loss and the formed metallonitrene can undergo C–H insertion reactions with aldehydes to give amides *via* nitrogen atom transfer.[2]

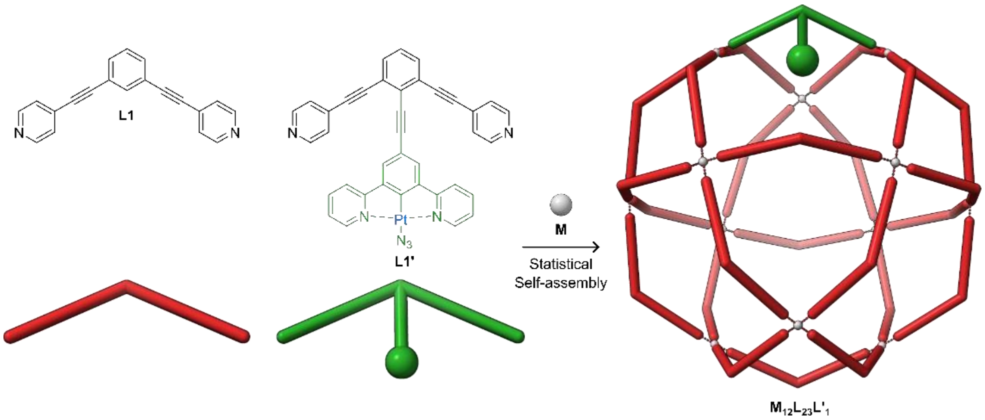

Figure 1: Example of a statistically self-assembled heteroleptic $M_{12}L_{24}$-$_x$L'$_x$ cage.

A library of ligands containing different chromophores will be synthesized and studied, to obtain light-harvesting cages that facilitate the light induced nitrene formation.

References:

[1] a) C. C. James, B. de Bruin, J. N. H. Reek, *Angew. Chem. Int. Ed.* **2023**, *62*, e202306645; b) A. C. Pearcy, J. D. Crowley, *Chem. Eur. J.* **2023**, *29*, e202203752

[2] a) T. Schmidt-Räntsch, H. Verplancke, J. N. Lienert, S. Demeshko, M. Otte, G. P. van Trieste, K. A. Reid, J. H. Reibenspies, D. C. Powers, M. C. Holthausen, S. Schneider, *Angew. Chem. Int. Ed.* **2022**, *61*, e202115626

Pyrene-based emitter materials for lasing and super-fast light emission

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Polycyclic aromatic hydrocarbons are frequently used as gain medium in organic lasers, due to their chemical tunability and large stimulated emission cross section.[1] Pyrene derivatives are promising candidates in optoelectronic devices, as their rigid molecular structure provokes excellent photoluminescence efficiency and high charge carries mobility combined with great hole injection ability.[2,3] However, there are only a few examples of pyrene gain materials and the tuneability of the lasing behavior through substituents is not yet examined and optimized. Here, we design simple blue emissive pyrene derivates with different substituted electron donors.

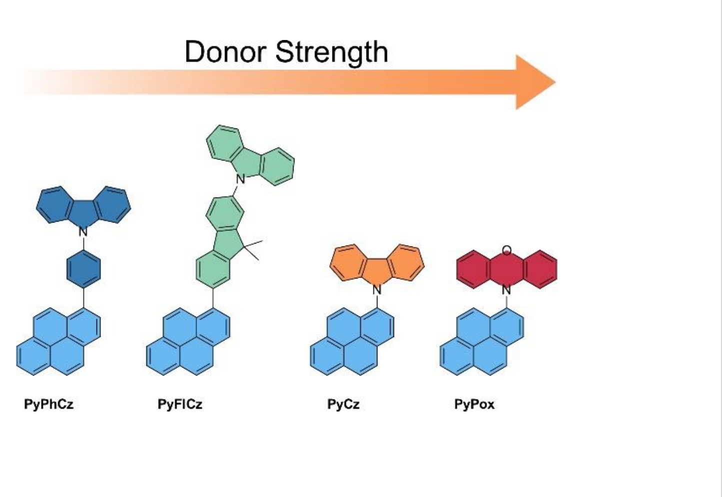

Figure: Structure of the examined pyrene-based compounds arranged according to the donor strength as determined by the dipole moment.

We investigate the influence of the electron donating substituents on the ability of pyrene derivatives to exhibit Amplified Spontaneous Emission (ASE) and observe low thresholds down to 1.73 µJ cm^{-2}. Through comprehensive spectroscopic and theoretical analysis, we outline the correlation between electron density and ASE threshold, emission efficiency, and excited state lifetime. Our results demonstrate that higher electron density inhibits ASE performance, attributed to the stabilization of excited states, while lowering the photoluminescence quantum yield.

References:

[1] A. J. C. Kuehne, M. C. Gather, *Chem. Rev.* **2016**, *116*, 12823–12864.
[2] L. Ma, Y. Yu, L. Li, T. Lei, B. Jiao, X. Hou, Z. Wu, *Org. Electron.* **2018**, *57*, 123–132.
[3] M. Fang, J. Huang, Y. Zhang, X. Guo, X. Zhang, C. F. Liu, W. Y. Lai, W. Huang, *Mater. Chem. Front.* **2017**, *1*, 668–676.

Intercalation of dicarboxylic acids into porous supramolecular nanopatterns on graphite (HOPG)

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Rigid entities consisting of ethynylene and phenylene units are of great interest due to their wide range of applications, including metal chelate ligands[1], enzyme transporters[2], molecular electronics[3], or surface studies.[4] One aspect of the latter deals with supramolecular nanopatterns, that form at the solid/liquid interface of a solution of an organic species and a solid material, such as highly oriented pyrolytic graphite (HOPG). Here, we report on the synthesis and self-assembly of an arylene alkynylene carrying two carboxylic acid units and 3,4,5-trialkoxybenzyloxy units (Figure 1). The former are prone to interact non-covalently, while the latter mediate sufficient compound solubility. When a solution of dicarboxylic acid (Figure 1, *left*), is applied to a porous supramolecular template layer of arylene-alkynylene macrocycles, cyclotrimers are found (Figure 1, *right*) in its nanopores, that act as a host. In all cases, the supramolecular adsorbate structures formed are visualized by scanning tunneling microscopy (STM) with submolecular resolution.

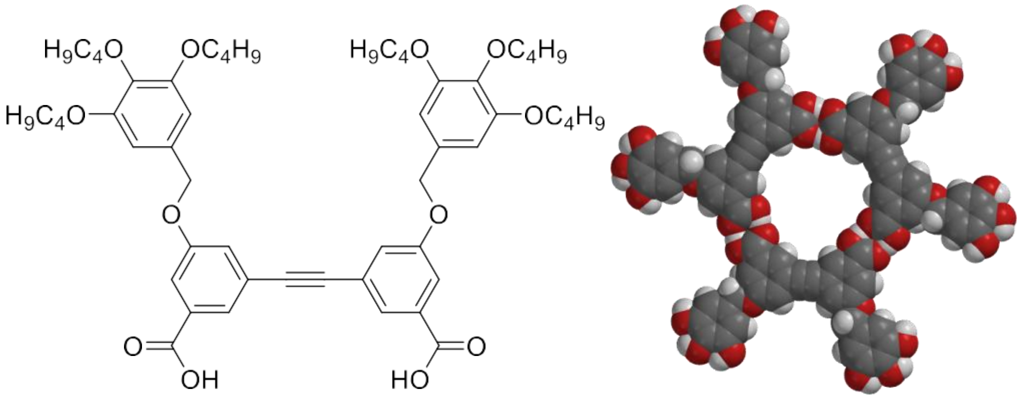

Figure 1: Dicarboxylic acid (*left*) and space-filling model of a supramolecular cyclotrimer thereof (*right*; alkoxy chains omitted for clarity).

References:

[1] Khatyr, A.; Ziessel, R. *J. Org. Chem.* **2000**, *65* (10), 3126-3134. DOI: 10.1021/jo9919355.
[2] Malolanarasimhan, K; Kedei, N; Sigano, D. M.; Kelley, J. A.; Lai, C. C.; Lewin, N. E.; Surawski, R. J.; Pavlyukovets, V. A.; Garfield, S. H.; Wincovitch, S.; Blumberg, P. M., Marquez, V. E. *J. Med. Chem.* **2007**, *50* (5), 962-978.
[3] Wielopolski, M.; Atienza, C.; Clark, T.; Guldi, D. M.; Martín, *Chem. Eur. J.* **2008**, *14* (21), 6379-6390.
[4] Jester, S.-S.; Sigmund, E; Höger, S. *J. Am. Chem. Soc.* **2011**, *133* (29), 11062-11065.

Photo cross linker for emulsion polymerization

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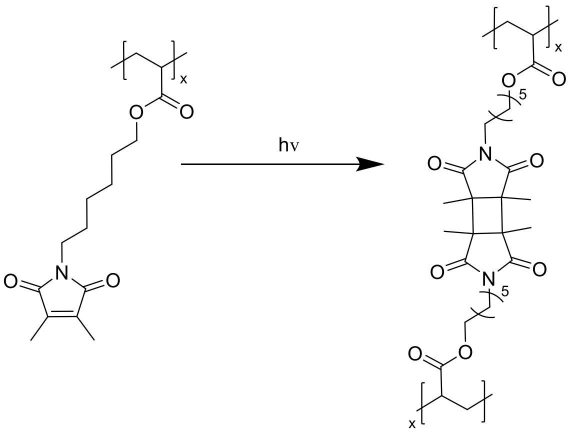
The current research area deals with the synthesis of photo cross linkers for emulsion polymerization. The topic follows on from the work of *C. Henschke*. The film of emulsion polymerization swells when drying or dissolves by contact with solvents. The photo cross-linker is intended to prevent this by cross-linking the polymer in a [2+2] cycloaddition through irradiation with UV light. For this purpose, the reactive cross-linking unit is pyrroldione, which can form stable dimers (Scheme 1).[1]



Scheme 1: Photo cross-linking reaction of P_{MT}1.[1]

The UV absorption of the cross linker **P_{MT}1** lies around 230 nm and 300 nm. This low wavelength potentially cleaves the polymer backbone, which lead to the idea of mixing thioxanthone to the polymer as photo sensitizer in order to enable photo cross-linking with wavelengths around 360 - 430 nm.[1]

References:

[1] D. Kuckling, M. E. Harmon, C. W. Frank, *Macromolecules* **2002**, *35*, 6377.

Endo-endo Bridged Ligand Pairs for Self-Sorting in $\mathrm{Pd_2L_4}$ Cages

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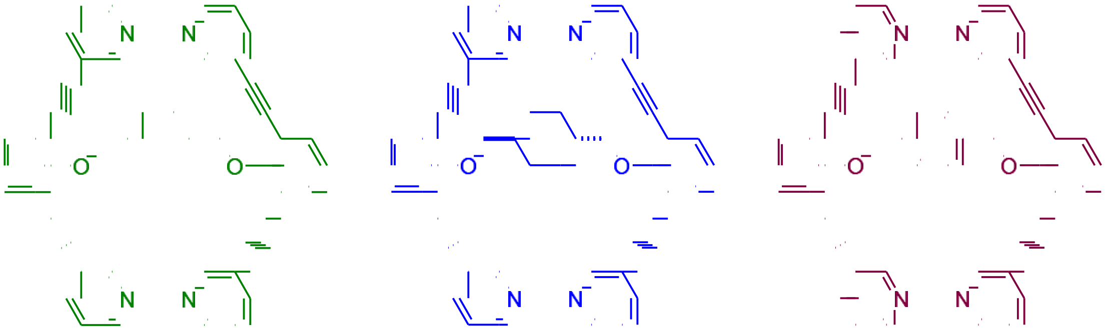
Self-assembly is one possible pathway for the formation of supramolecular structures from smaller building blocks. In addition to this, reliable methods for self-sorting are indispensable for the successful design and synthesis of more complex heteroleptic cages. Steric bulk[1] and shape complementarity[2] can for example be used to achieve self-sorting. Herein we present a new method of self-sorting currently under development: *endo-endo* bridging of ligand pairs. Hereby formed complexes should exhibit a higher stability and this method would enable the formation of complexes containing similar ligands with differently functionalized backbones, thereby opening the doors to a variety of applications for chromophore-decorated ligands.



$L_2B_{n\text{-hex}}$ **L_2B_{cyhex}** **L_2B_{ph}**

Figure 1: Synthesized, easily accessible, *endo-endo* bridged ligand pairs with an increasing bridge rigidity.

Preliminary studies indicate an increased bridge rigidity favors the formation of heteroleptic $\mathrm{Pd_2L_2(L_2B)}$-type complexes.

References:

[1] Q. Zhang et al. *Angew. Chem. Int. Ed.* **2023**, *62*, e202217215.
[2] G. H. Clever et al. *Nat. Chem.* **2024**, *16*, 584–591.

Circularly Polarized Luminescence and Supramolecular Interactions of Diketo[9]CPP and DBP[9]CPP

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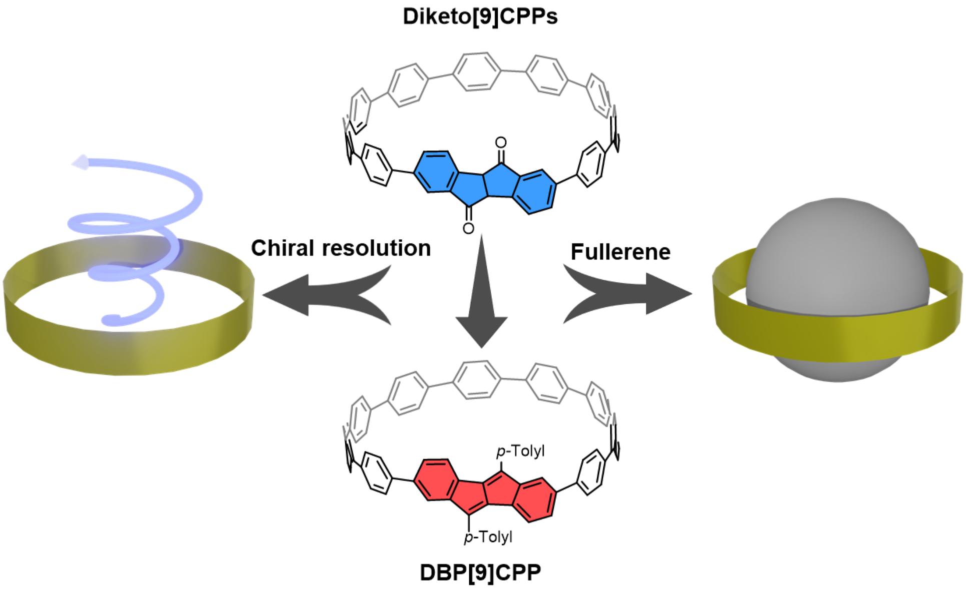
Cycloparaphenylenes (CPPs) exhibit unique physical and chemical properties, making them promising materials for various fields, such as materials science, electronics, and biological applications. [1,2]

Our previous work involved synthesizing diketo[7]CPP, which showed good chiroptical properties and structural flexibility.[3] Building upon this work, we synthesized larger nanohoops (Diketo[9]CPP and DBP[9]CPP) and investigated those compounds for potential utilization in the fields of circularly polarized luminescence (CPL) materials and supramolecular chemistry.



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