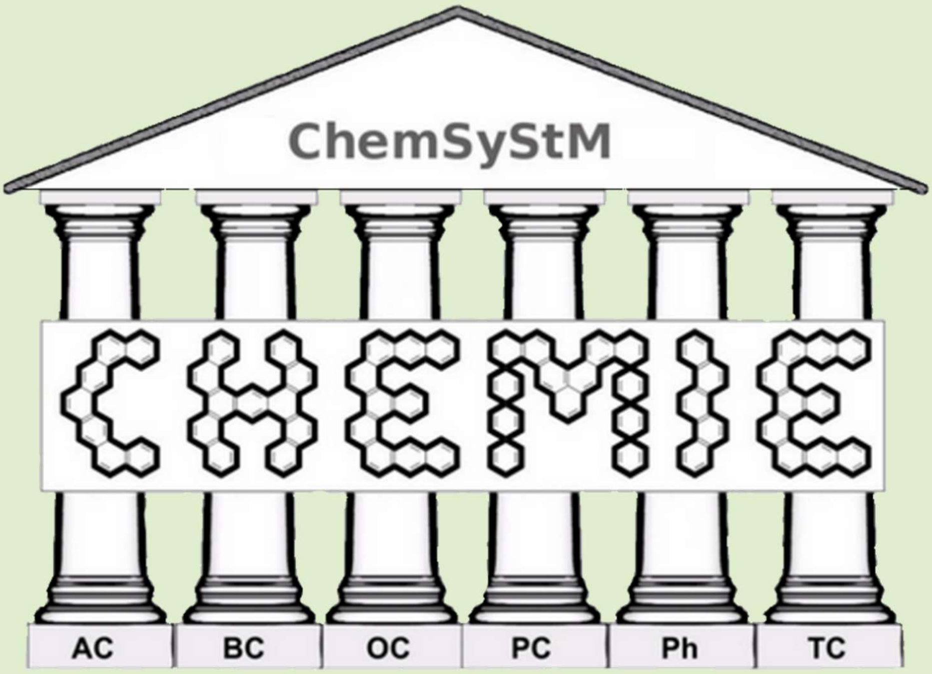
ChemSyStM 2025



das 9te Chemie-Symposium der Studierenden Mainfrankens

Abstractband

GDCh
JCF
Würzburg

02.12.2025

https://jcf.io/wuerzburg

Inhaltsverzeichnis des Abstractbandes

Dieser Abstractband besitzt keine Seitenzahlen. Dafür sind jeweils am Rand die Posternummern eingetragen. In eben dieser Reihenfolge sind die Poster auch während der Posterpräsentation aufgestellt. Weitere Informationen können aus den Teilnehmerlisten entnommen werden.

Grußwort JCF

Liebe Teilnehmer der ChemSyStM 2025, sehr geehrte Gäste,

voller Freude begrüßen wir Sie zum mittlerweile 9ten Chemie Symposium der Studierenden Mainfrankens. Nachdem unser Symposium im vergangenen Jahr seinen achtzehnten Geburtstag und damit seine Volljährigkeit feiern konnte, schauen wir voller Stolz auf vergangene Jahre zurück und blicken zuversichtlich in eine Zukunft in der Dialog und wissenschaftlicher Diskurs essentieller sind denn je.

Gleichsam der vergangen Jahren ist es dieses Jahr das Anliegen des JCFs den wissenschaftlichen Austausch an unserer Universität zu fördern und in einer familiären Atmosphäre die wissenschaftliche Neugier auch über die Grenzen des eigenen Fachbereiches zu wecken. Wie auch in den vergangenen Jahren steht im Zentrum der ChemSyStM die Studierendenschaft, ohne deren Zutun ein derartiger Austausch und Kontakt nicht möglich wäre, da ein jeder einzelne Beitrag maßgeblich zum Erfolg dieses Symposiums und zur wissenschaftlichen Zukunft unserer Universität beiträgt.

Als Appetitanreger dienen die Poster-Appetizer zu Beginn der ChemSyStM, welche einen Vorgeschmack auf die folgenden Posterpräsentationen bieten sollen. Der im Anschluss stattfindende Vortrag des VAA erlaubt einen Blick auf die Zeit nach der studentischen Laufbahn und auf den Einstieg ins Berufsleben. Im Mittelpunkt der Veranstaltung steht die Posterpräsentation. Diese bietet die Möglichkeit in vertrautem Umfeld erste oder weiterführende Fertigkeiten im wissenschaftlichen Präsentieren und Kommunizieren zu erlangen und neue Kontakte knüpfen zu können. Seinen Ausklang findet die Veranstaltung im Abendvortrag von Herr Dr. Kunz zum Thema „Plastikmüll: Wissen und Spekulation".

Abschließend wünscht euch das JCF Würzburg viel Erfolg und Spaß auf der ChemSyStM 2025 und hofft auf einen regen und lebendigen Austausch und eine angenehme Veranstaltung.

Euer Sprecher des JCF-Würzburgs

Jonas Seifert

Grußwort OVV

Als Ortsverbandsvorsitzender der GDCh Unterfranken heiße ich Sie alle herzlich zur diesjährigen ChemSyStM willkommen. Es freut mich außerordentlich, dass das JungeChemieForum diese traditionsreiche Veranstaltung erstmals seit 2022 wieder aufleben lässt – mit einem spannenden Programm aus metaphorischen und kulinarischen Poster-Appetizern, einer Postersession und einem vielversprechenden Abendvortrag.

Diese Veranstaltung lebt davon, Gewissheiten nicht einfach hinzunehmen – ein Gedanke, der sich im provokanten Bonmot von Richard Feynman spiegelt: Wissenschaft sei der Glaube an die Unwissenheit der Experten. Dies stellt keinesfalls eine Geringschätzung von Expertenwissen dar, sondern erinnert vielmehr daran, dass wissenschaftliches Verständnis immer vorläufig ist und stetem Wandel unterworfen bleibt. Fortschritt entsteht dort, wo es gelingt, bestehende Annahmen konsequent durch neue Evidenz in Frage zu stellen.

Die Fähigkeit dazu erwerben Sie in Praktika, im Labor und im Alltag Ihres Studiums – im Diskurs, durch Zuhören, Verstehen und Entgegnen. Die ChemSyStM bietet einen idealen Rahmen, um das, was Sie bislang gelernt und geleistet haben, zur Schau und auf die Probe zu stellen.

Postersitzungen sind ein dafür besonders geeignetes Format. Für mich persönlich verbinden sich mit ihnen einige der prägendsten Erinnerungen meiner wissenschaftlichen Laufbahn: überraschende Gespräche, neue Ideen, gemeinsames Nachdenken – und nicht selten auch neue Freundschaften haben hier ihren Anfang.

Wenn ich den Studentinnen und Studenten meiner Forschungsgruppe gelegentlich erkläre, eine der wichtigsten Qualifikationen, die sie aus dem Studium mitnehmen, sei Frustrationstoleranz, dann ist das zwar wahr, aber auch bewusst zugespitzt. Ebenso essenziell ist es, Gelegenheiten wie die ChemSyStM zu nutzen, um den wissenschaftlichen Austausch mit Gleichgesinnten zu pflegen, eigene Hypothesen zu prüfen und neue Perspektiven zu gewinnen.

In diesem Sinne wünsche ich Ihnen eine lebendige, erkenntnisreiche und inspirierende Veranstaltung – mit guten Gesprächen, klaren Argumenten und bleibenden Eindrücken.

Prof. Dr. Tobias Hertel
Ortsverbandsvorsitzender der GDCh Unterfranken

Grußwort Dekan

Liebe Studierende und Gäste der ChemSyStM,

das Chemie Symposium Studierender Mainfrankens, kurz ChemSyStM ist in der mittlerweile neunten Auflage schon zu einer gut gepflegten Tradition an der Fakultät für Chemie und Pharmazie geworden.

Der nachhaltige Erfolg dieser Veranstaltung beruht vor allem auf ihrem interdisziplinären Charakter. Die ChemSyStM bringt Forschende aus allen Bereichen unserer Fakultät zusammen und fördert einen offenen wissenschaftlichen Austausch über Instituts- und Fachgrenzen hinweg. Insbesondere für Studierende im Bachelor- und Masterstudium stellt das Symposium eine wertvolle Gelegenheit dar, Einblicke in die vielfältigen Forschungsthemen an der Universität Würzburg zu gewinnen und sich schon vor einem möglichen Promotionsstudium aktiv in den wissenschaftlichen Dialog einzubringen.

Mein besonderer Dank gilt dem engagierten Team des JungenChemieForums (JCF), deren ehrenamtlicher Einsatz das exzellente wissenschaftliche Angebot unserer Universität auf vielfältige Weise bereichert. Ebenso danke ich allen Teilnehmenden und den großzügigen Sponsoren, die dieses Symposium ermöglichen und unterstützen.

Ich wünsche allen Beteiligten ein inspirierendes Symposium, anregende wissenschaftliche Diskussionen und wertvolle neue Perspektiven.

Herzlichst

Ihr

Holger Helten

(Dekan der Fakultät für Chemie und Pharmazie)

Programm der ChemSyStM

12.15 Uhr	Begrüßung mit Vorstellung
12.30 Uhr	Poster- Appetizer
13.30 Uhr	Pause (Kaffee und Kuchen)
14.00 Uhr	Vortrag VAA
15.00 Uhr	Poster- Session
17.30 Uhr	Abendvortrag von Herr Dr. Kunz Plastikmüll: Wissen und Spekulation mit anschließender Preisverleihung

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Sponsoren der ChemSyStM 2025

Ein herzliches Dankeschön für die Unterstützung und das Vertrauen an:

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Chemie

Verband für Fach- und Führungskräfte in der chemisch-pharmazeutischen Industrie (VAA)

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Poster-Appetizer

#	Nachname	Vorname	Arbeitskreis	Kategorie
25	Chorbacher	Johannes	Helten	Anorganische Chemie
3	Farn	Nikolas	Höbartner	Organische Chemie und Pharmazie
7	Hofmann	Klaus	Fischer	Physikalische und Theoretische Chemie
18	Heldner	Maxi Liesa	Hierlmeier	Anorganische Chemie
22	Lutz	Sarah	Helten	Anorganische Chemie
39	Schittenhelm	Lena	Unterlass	Funktionswerkstoffe und Chemiedidaktik
24	Ma	Chenchang	Ye	Anorganische Chemie
27	Miao	Xincheng	Mitrić	Physikalische und Theoretische Chemie
31	Kolla	Sai Teja	Wencel-Delord	Organische Chemie und Pharmazie
38	Sailer	Frank	Unterlass	Funktionswerkstoffe und Chemiedidaktik

1

N-HETEROCYCLIC SILYLENE COMPLEXES OF NICKEL(0)

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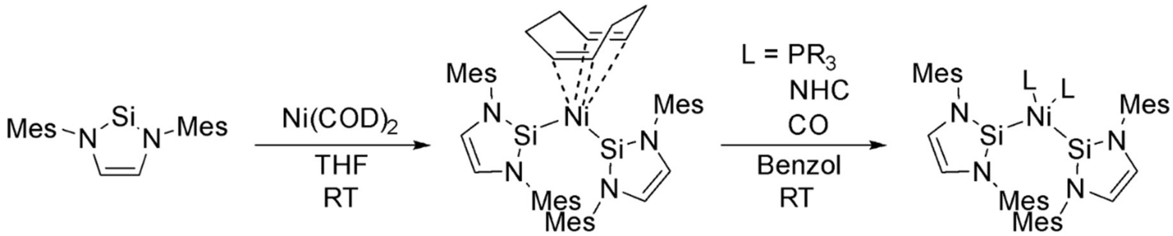
Since the discovery of the first *N*-heterocyclic carbene in **1991** through Arduengo a multitude of novel NHC-metal-complexes had been synthesized and characterized.[1] In comparison, for *N*-heterocyclic silylenes, which were discovered in **1994** by Denk/West, only a few transition metal complexes are known in the literature.[2] We previously reported the synthesis and characterization of Dipp$_2$NHSi transition metal complexes, observing a different reactivity compared to the isostructural NHCs.[3] NHCs exclusively show terminal coordination to the metal center, whereas NHSi ligands can also insert into the metal halide M-X bond or act as bridging ligands between two metal centers. Herein, we wish to report the synthesis and characterization of mesityl-substituted NHSi nickel-complexes [Ni(Mes$_2$NHSi)$_2$L$_2$] (L = PMe$_3$, PEt$_3$ PBu$_3$, IMe$_4$, CO) (see Scheme 1)[4] and trigonal coordinated nickel complexes [Ni(Mes$_2$NHSi)$_2$(NHC)] and [Ni(Mes$_2$NHSi)(NHC)$_2$] (NHC = I*i*Pr^{Me}) starting from the COD-substituted *bis*-NHSi nickel-complex.[5]



Scheme 1: Synthesis route of *bis*-NHSi substituted nickel-complexes.

References

[1] A. J. Arduengo, R. L. Harlow, M. Kline, *J. Am. Chem. Soc.* **1991**, *113*, 361-363J Am Chem Soc.

[2] M. Denk, R. K. Hayashi, R. West, *J. Chem. Soc., Chem. Commun.* **1994**, 33-34.

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[4] E. Glok, L. Werner, U. Radius, *Dalton Trans.* **2025**, Advance Article.

[5] L. Kong, J. Zhang, H. Song, C. Cui, *Dalton Trans.* **2009**, 5444-5446.

2

Anionic Carbenes as Ligands in Main Group and Transition Metal Chemistry

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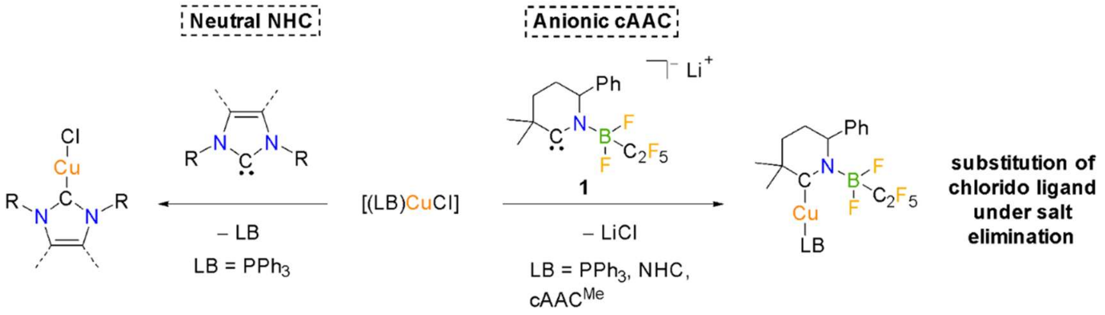
In the last decades *N*-heterocyclic carbenes and cyclic (alkyl)(amino) carbenes emerged as considerable alternative to commonly used phosphines as ancillary ligands in transition metal chemistry.[1] Since the development of novel anionic borane-substituted *N*-heterocyclic carbenes (anionic NHCs)[2] and cyclic (alkyl)(amino)carbenes (Ani-cAACs)[3], we have investigated their reactivity and the modulation of their electronic and steric properties.

In this work, we report on the synthesis of the linear Ani-cAAC-substituted copper(I) complexes. The reaction of Ani-cAAC **1** with the copper(I) complexes [(LB)CuCl] (LB = PPh_3, NHC, $cAAC^{Me}$) resulted in the substitution of the chlorido ligand under salt elimination, leading to the formation of linear complexes of the type [(LB)Cu(Ani-cAAC-$BF_2(C_2F_5)$)]. Noteworthy, no substitution of the neutral *Lewis* base was observed.



Scheme 1: Reaction of linear copper(I) complexes [(LB)CuCl] with neutral NHC *vs.* Ani-cAAC **1**.

To expand the scope of anionic NHCs, we synthesized the borane-substituted 1-isopropyl-3-(tricyanoborane)-imidazolin-2-ylidenate anion and the 1-isopropyl-3-(pentafluoroethyldifluoroborane)-imidazolin-2-ylidenate anion in high yields. The properties of these compounds and data derived from theoretical calculations provide an insight into the electronic and steric properties of these novel anionic NHCs. The simplicity of the synthesis, along with properties such as negative charge, strong *σ*-donor and *π*-acceptor abilities, make anionic NHCs distinctive and promising building blocks in transition metal chemistry.

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[2] a) L. Zapf, U. Radius, M. Finze, *Angew. Chem., Int. Ed.* **2021**, *60*, 17974-17980; *Angew. Chem.* **2021**, *133*, 18118-18125, b) L. Zapf, S. Peters, R. Bertermann, U. Radius, M. Finze, *Chem. Eur. J.* **2022**, *28*, e202200275.

[3] L. Zapf, S. Peters, U. Radius, M. Finze, *Angew. Chem., Int. Ed.* **2023**, *62*, e202300056; *Angew. Chem.* **2023**, *135,* e202300056.

3

RNA-catalyzed synthesis of prenylated RNA

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Natural RNA modifications, commonly summarized as epitranscriptomics, constitute an additional structural and informational layer of RNA beyond four canonical nucleotides. Hitherto, more than 170 natural modifications have been reported. Though RNA modifications significantly shape the structure and function of RNA and are essential for variety of cellular biochemical processes including gene expression, splicing and translation, the detailed mechanisms of action, regulation pathways, and interaction partners of them remain poorly studied. Targeted artificial RNA modifications are required for structural and functional interrogation of natural RNAs. Catalytic RNAs – ribozymes – are emerging tools for site-specific modification of RNA advancing the toolset for such RNA modifications on purpose[1,2]. In our study, we use the alkyltransferase ribozyme MTR1 for targeted site-specific installation of naturally occurring prenylated adenosine modifications as well as their structurally related artificial analogues into the RNA of interest. Notably, the scope of RNA substrates spreads over natural motifs and includes highly structured sequences like tRNAs. Our RNA modification approach acts in a highly programmable manner and potentially enables structural and functional elucidation of natural modifications in their natural sequence context. In addition, we examined the mechanism of ribozyme-catalyzed prenylation reaction by kinetic isotope effect (KIE) measurements revealing new insights about the *modus operandi* of ribozymes.

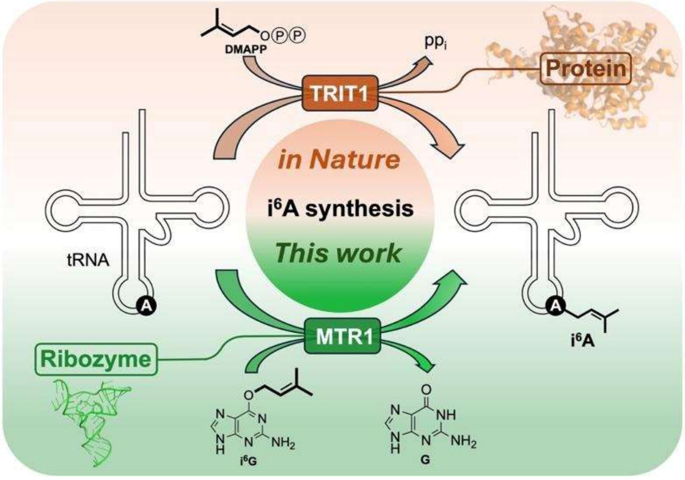

Figure 1: Graphical abstract.

[1] C. P. M. Scheitl, M. Ghaem Maghami, A-K. Lenz, C. Höbartner, *Nature* **2020**, 587, 663–667.
[2] M. B. Walunj, C. P. M. Scheitl, T. Jungnickel, C. Höbartner, *Angew. Chem. Int. Ed.*, **2025**, e202500257.

Neue experimentelle Alleskönner für das Thema Farbstoffe: DASAs

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Farbstoffe im Chemieunterricht werden in der Regel an klassischen Vertretern wie Indigo oder Azofarbstoffen besprochen, die unbestritten Bedeutung in der chemischen Synthese und industriellen Anwendung besitzen. Allerdings gibt es nur wenige für Schulen mögliche bzw. zugelassene Synthesen oder Handversuche. Die Durchführbarkeit im schulischen Zusammenhang wird dadurch eingeschränkt, dass viele Reaktionswege zu komplex oder die Ausgangsstoffe zu teuer und gefährlich sind.

Um diesen Herausforderungen zu begegnen und um die Bandbreite an experimentellen Möglichkeiten beim Thema *Farbstoffe* zu erweitern, wird eine völlig neue Farbstoffklasse für den schulischen Einsatz vorgestellt: die Donor-Akzeptor Stenhouse Addukte (DASAs). Diese innovativen Verbindungen wurden vor ca. 10 Jahren erstmals synthetisiert [1] und zeichnen sich durch einen modularen Aufbau aus, der es erlaubt, eine Vielzahl an chemischen Prinzipien von Farbstoffen anhand eines einzigen Systems zu veranschaulichen.

Ein wesentlicher Vorteil der im Poster vorgestellten DASA-Synthese liegt in der leichten Durchführbarkeit. Die Reaktionen erfordern keine aufwändigen Apparaturen, da sie primär im wässrigen Milieu ablaufen. Der Einsatz von organischen Lösungsmitteln wird auf ein Minimum reduziert. Zudem sind die verwendeten Edukte vergleichsweise günstig. Die einfache Handhabung und die ökologisch wie ökonomisch vorteilhafte Methodik machen diese DASAs zu einem besonders attraktiven Beispiel für schulische Synthesen.

Darüber hinaus bieten DASAs aufgrund ihrer stimuliresponsiven Eigenschaften – etwa bezüglich Licht, Acidität und Polarität – affektiv wirksame Farbphänomene und damit mögliche Zugänge zur Untersuchung der zugrundeliegenden Mechanismen. Schülerinnen und Schüler können anhand der DASAs experimentell erforschen, wie äußere Stimuli zu Veränderungen im Farbspektrum führen, und dabei wichtige Konzepte wie Elektronendonor- und -akzeptorwechselwirkungen oder die Wirkung von Lösungsmittelparametern praktisch nachvollziehen. [2]

Darüber hinaus erlaubt der modulare Aufbau der DASAs eine umfassende Integration schulrelevanter Prinzipien im Zusammenhang mit Farbstoffchemie, z.B. Konjugationssysteme und (anti-)auxochrome Gruppen. Durch Einbeziehen der aktuell sehr aktiven Forschung zu DASAs können Lernende nicht nur traditionelle Inhalte wiederholen, sondern auch Einblicke in den dynamischen Charakter der naturwissenschaftlichen Forschung erhalten (*nature of science*). Daran anknüpfend wurden im Rahmen der Arbeit neue Ansätze für den schulgeeigneten Einsatz fachtypischer Arbeitsweisen beim Thema Farbstoffe demonstriert.

[1] Clerc, M.; Sandlass, S.; Rifaie-Graham, O.; Peterson, J. A.; Bruns, N.; Alaniz, J. R. de; Boesel, L. F. *Chem. Soc. Rev.* **2023**, *52* (23), 8245–8294.

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5

A Very New metal complexes for ruthenium-based photoactivated chemotherapy (PACT)

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Ruthenium-based photoactivated chemotherapy (PACT) refers to compounds that exhibit the ability to undergo a photosubstitution reaction with various solvents such as water, acetonitrile, or DMSO, with the resulting photoproduct then triggering cell death.[1]

Supported by theoretical calculations, it was shown that variation of the ligands in octahedral ruthenium complexes influences the photoactivation wavelength range.[2]

In this study, ruthenium-based [3+2+1] complexes were designed as novel potential PACT agents, to have their photoactivation range shifted to the red-light part of the spectrum. The monodentate ligand, which so far was mostly neutral, has been changed to a triazolato species in this new approach, which is then to be photosubstituted and released.

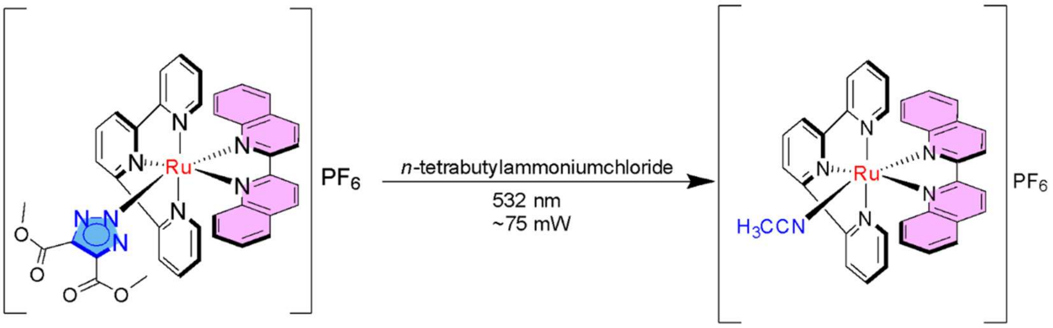

Figure 1: Ligand substitution in a [3+2+1] Ru(II) triazolato complex by green light as a novel approach to PACT

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6

Kontextorientierte Experimente zur NMR-Spektroskopie für die Lehramtsausbildung

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NMR-Spektroskopie (engl. nuclear magnetic resonance, kernmagnetische Resonanz) ist eine der wichtigsten Analysemethoden in der modernen chemischen Forschung. Allerdings gilt NMR-Spektroskopie als schwierig zu lehren und lernen, wobei spezifischere empirische Untersuchungen zu diesem hochschuldidaktischen Thema fehlen.[1] Insbesondere der Einsatz von Experimenten zur NMR-Spektroskopie ist wenig untersucht. Dies liegt unter anderem an den hohen Anschaffungs- und Wartungskosten von NMR-Spektrometern. Speziell Lehramtsstudierende der Chemie sammeln daher in ihrem Studium kaum Erfahrungen mit NMR-Experimenten, obwohl dies in den Stoffkatalogen der Gesellschaft Deutscher Chemiker (GDCh) und der Kultusministerkonferenz der Länder (KMK) gefordert wird.[2,3]

Seit etwa 15 Jahren gibt es jedoch kompakte Benchtop-NMR-Spektrometer, die auf der Grundlage von Permanentmagneten im Niedrigfeld-Bereich arbeiten. Sie zeichnen sich durch geringere Kosten sowie eine einfache Handhabung aus und eignen sich deswegen für den Einsatz in der Hochschullehre.[4]

Im Rahmen meiner Promotion wurden für diese Spektrometer Experimente entwickelt, die sich im Chemie- und Lehramtsstudium in einem Hochschulpraktikum einsetzen lassen. Der Fokus lag dabei darauf, kontextualisierte Versuche zu konzipieren, die an bestehendes Alltagswissen der Studierenden anschließen können. Zum Kontext Alkohole wurden daher Experimente entwickelt, mit denen sich die Grundlagen der NMR-Spektroskopie anhand der Spektren einfacher Alkohole vermitteln lassen. Säfte und Spirituosen eignen sich für qualitative und quantitative Analytik mittels NMR-Spektroskopie. In Fruchtsäften lassen sich Art und Menge verschiedener Zucker nachweisen, in Spirituosen kann der Methanol- und Ethanolgehalt bestimmt werden. Der Prozess der alkoholischen Gärung bietet einen Einstieg in die Verfolgung chemischer Reaktionen (Reaction monitoring). Die Hydrolyse von Saccharose als Teilschritt dieser biochemischen Reaktion eignet sich für tiefgreifendere kinetische Untersuchungen. Daneben wurden auch weitere einfache chemische Reaktionen und deren Kinetik analysiert. Mit dem verwendeten Benchtop-Spektrometer und den entwickelten Methoden ließen sich Ergebnisse erzielen, die im Bereich der Literatur- und Referenzwerte liegen.

Eine didaktische Aufarbeitung dieser Experimente wurde im Rahmen eines Hochschulpraktikums an der Universität Würzburg durchgeführt und evaluiert. Das fachliche und fachdidaktische Wissen der Studierenden nahm im Laufe des Praktikums zu und es zeigte sich, dass kontextualisierte Versuche das Interesse an NMR-Experimenten wecken können. Zusätzlich wurde eine Schülerlaborstation erarbeitet und evaluiert. Dabei wurde deutlich, dass auch Schülerinnen und Schüler die Grundideen der NMR-Spektroskopie verstehen und sich für dieses moderne Messverfahren begeistern können. Mit dieser Arbeit steht somit eine experimentelle Erarbeitung der NMR-Spektroskopie für verschiedene Lerngruppen zur Verfügung.

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Investigation of Chiral Molecules Using Raman Optical Activity

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Raman Optical Activity (ROA) is a type of spectroscopy to detect chirality in solutions. Like circular dichroism, signal differences are measured utilizing circular polarized light. The resulting spectrum in the vibrational regime gives information about the molecular geometry and environment of the sample, which can be analysed by comparing it with quantum chemical calculations.[1]

ROA spectra exhibit high levels of noise and are prone to spurious signals, since the intensity difference is roughly 0.1% of the corresponding Raman peak which itself is only 0.0001% of the incident light. To overcome these challenges, a Raman spectrometer was custom-built and modified to detect ROA.[2]

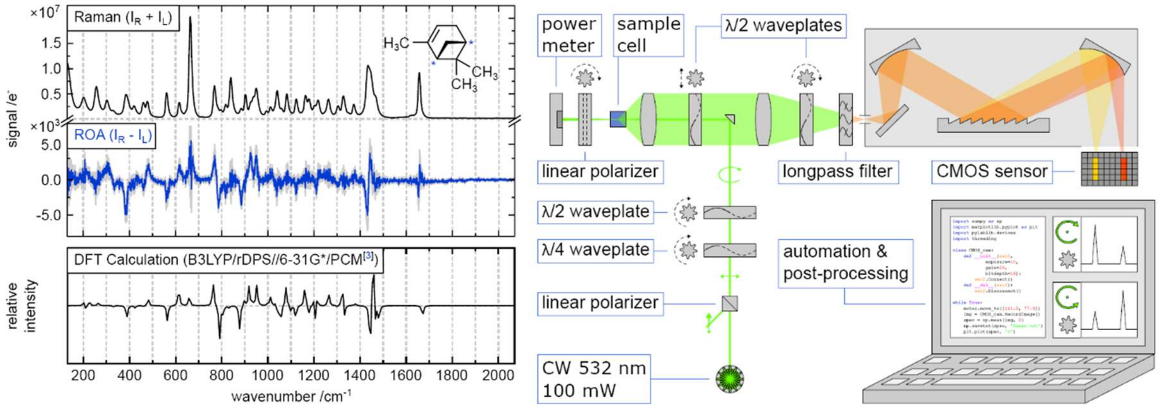

Figure 1: Beam path of the custom-built ROA spectrometer and recorded ROA spectrum of (−)-α-pinene.[2]

The setup was built using commercially available, cost-efficient components and a lot of efforts. Waveplates were introduced to convert linear to circular polarized light, which is repeatedly switched between left- and right-handed polarization by motorized mounts. Python was used to automate the experiment, data acquisition and post-processing to obtain the Raman difference spectrum. For the validation of the obtained results, the recorded ROA spectrum of (−)-α-pinene is compared to DFT calculations.[3]

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8

SHOWCASING THE DANCE OF PHOSPHOGLYCOLATE PHOSPHATASE (PGP): PROTEIN CONFORMATIONAL CHANGES GUIDING THE FINDING OF NEW INHIBITORS

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Misleading phosphorylation and dephosphorylation can lead to several diseases. The sizeable superfamily of haloacid dehalogenase (HAD) phosphatases has gained increasing pharmacological interest over the last decade.[1] As a member, phosphoglycolate phosphatase (PGP), a metabolite damage control enzyme with the ability to dephosphorylate and repair adventitious glycolytic metabolites,[2-4] has been proven as a pharmacologically actionable target.[5] Nevertheless, its potential to target, for instance, autoimmune responses and cancer diseases remains untapped. Therefore, new inhibitors are needed to further explore PGP as a therapeutic target.

Combining molecular modeling, docking, and molecular dynamics simulations, we shed light on the protein conformational changes and behavior of PGP upon interaction with specific small-molecule inhibitors. We illustrate a computational journey starting from the first X-ray crystal structures of an inactive mutant of murine PGP[5] (in the absence and presence of the hitherto most potent inhibitor) to the identification of subtle conformational changes (of the catalytically active PGP) as well as protein-ligand interactions essential for its inhibition. These findings were sustained by further studying the "molecular dance" behind the crystallographic data of human PGP with a newly found inhibitor, providing a more plausible basis for improving PGP inhibitors via computer-aided molecular design.

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9

To React or not to React – the Structural Investigation of the Alkyltransferase Ribozyme SAMURI

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Structures determine functions—a concept holds true not only for proteins but also for nucleic acids. Despite having a much smaller repertoire of building blocks (A, C, G, U) compared to proteins, RNAs can fold into complex 3D structures, which renders them versatile functions in nature as well as in the laboratory. Riboswitches, for instance, are natural RNAs that sense the abundance of cognate metabolites and regulate gene expression through structural alterations. Ribozymes are another example of natural catalytic RNAs that mostly account for RNA cleavage or splicing. Through in vitro selection (or SELEX), numerous artificial ribozymes have been identified to catalyze diverse chemical reactions, among which alkyltransferase ribozymes are drawing increasing attention due to their high efficiency and selectivity to install RNA modifications, as demonstrated by the first methyltransferase ribozyme MTR1.[1]

Our group recently reported another alkylating ribozyme, SAMURI, which utilizes *S*-adenosylmethionine (SAM) or its selenium analogue (ProSeDMA) as cofactors to attach different alkyl groups on RNA with high selectivity and efficacy.[2] To understand the reaction mechanism, crystal structures were solved to 2.9 Å for both SAM-SAMURI and ProSeDMA-SAMURI complexes, revealing the post-catalytic structures with discharged cofactors (SAH or SeDHA) bound in the catalytic cores.[3] The 17-nt catalytic core folds into an architecture of 4 parallel layers, stabilized by continuous π-stacking and hydrated magnesium ions. The kink structure – a sharp turn in the substrate RNA – inserts the target nucleotide in the proximity of the cofactor and thereby facilitates the alkyl-transfer reaction through an S_N2-like mechanism. The SAMURI structures not only allowed us to optimize the cofactor structure to improve stability but also enables the structural comparison of two SAM-involving RNAs – SAM riboswitches and SAMURI. While SAM riboswitches strategically avoid placing nucleophiles near the sulfonium center of SAM to circumvent undesired self-methylation, SAMURI actively recruits SAM to the susceptible target to yield methylated RNA. Our study provides insights into the relationship of ribozymes and RNA modifications that may have been of importance in a putative primordial RNA world.

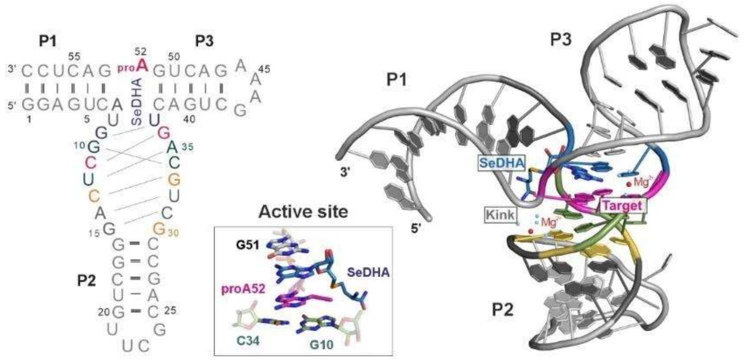

Figure 1: The overall structure of SAMURI and the zoom-in view of the active center.

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Cell Surface Engineering using Heterotelechelic RAFT-Polymers

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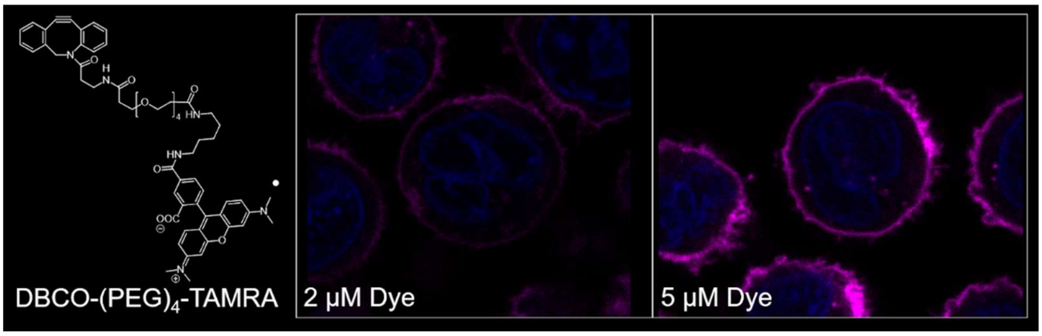
In recent years, the development of advanced biomaterials for cell surface modification has gained significant attention, particularly with the aim of enhancing cell interactions during biofabrication processes. A promising approach in this area is the use of multifunctional heterotelechelic polymers. They enable a precise functionalization of surfaces and can also be translated to cells as biological "living" substrates. This can e.g. facilitate controlled cell-cell interactions for advanced biofabrication models.

Well-defined polymers with heterotelechelic end groups can be accessed by RAFT polymerization using trithiocarbonates as chain transfer agents (CTAs) [1-4]. By employing a CTA reagent with a pentafluorophenyl attached, different monoamine-functionalized lipid anchors or clickable dibenzocyclooctynes can be installed onto the same polymer platform after polymerization. Customized poly(*N*,*N*-diacrylamide)s can be produced providing similar non-adhesive stealth properties as polyethylene glycol [1-3]. Alternative (co)polymerizations with e.g. glycosylated acrylamides provide access to glycocalyx mimics [4].

To study cell surface retention, the trithiocarbonate end groups can further be (reversibly) modified into thioether- or disulfide-modified species [1-3]. They can be applied to install fluorophores on the cell surface. Alternatively, copolymerization with dye-labeled arylate monomers can provide similar features but allows for additional end group modifications e.g. with biotin units for directed adhesion through streptavidin crosslinking or for targeted immobilization of growth factors.



In summary, we present a promising platform for heterotelechelic RAFT polymers in cell surface engineering, where precise chemical optimization can enable customizable controlled cell surface advancing the rising field of advanced biofabrication processes, explored by the interdisciplinary research center TRR225 (https://trr225biofab.de).

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11

The x-ray absorption spectrum of the *tert*-butyl radical

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Hydrocarbon radicals play an important role in atmospheric chemistry and combustion processes. They have been detected in interstellar space where they are key intermediates for the formation of complex species. However, spectroscopic information on radical species in the x-ray regime is scarce.

Here we present an investigation of the *tert*-butyl radical C_4H_9 by x-ray absorption spectroscopy (XAS), where carbon 1s electrons are excited into unoccupied orbitals (Figure 1a).

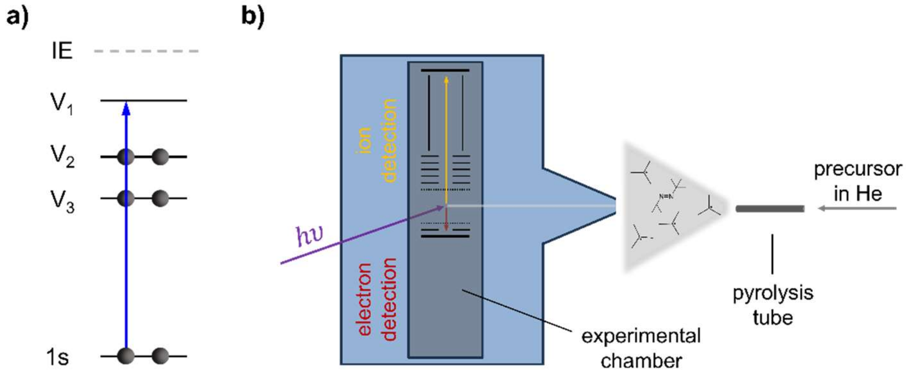

Figure 1: a) Scheme of the electronic process in x-ray absorption spectroscopy: Core electrons are excited into unoccupied molecular orbitals. b) Experimental setup: A pyrolysis source is coupled to an apparatus for electron-ion detection.

For open shell species this method is able to probe transitions into a singly occupied molecular orbital. The experiments were performed at the soft x-ray beamline GASPHASE at the synchrotron Elettra where electrons and ions resulting from the same ionization process are detected in coincidence (Figure 1b). The *tert*-butyl radical was generated by pyrolysis of azo-*tert*-butane and the spectrum of the pure radical was obtained by the subtraction of spectra measured at different temperatures. The lowest energy signal is assigned to the excitation of the 1s electron at the central carbon into the SOMO. Transitions of the terminal C1s electrons are shifted to higher energies. The signals in the XAS were assigned by *ab initio* calculations that show a very good agreement with the experimental data. Furthermore, we investigated the fragmentation of the core excited molecule for the excitation at different photon energies and identified the different fragmentation products.

12

Investigating Photoinduced Dynamics of a 1,4-Azaborine with Time-Resolved X-ray Spectroscopy

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Azaborines are molecules containing boron and nitrogen, exhibiting distinctive electronic properties by replacing carbon-carbon bonds in organic frameworks. This makes them promising candidates for applications in energy and electronic materials, such as optoelectronics and singlet fission systems.[1] In this study, the ultrafast dynamics of the non-commercial compound **1,4-*di*-*tert*-butyl-azaborine** were investigated using **time-resolved X-ray photoelectron spectroscopy**. The experiments were carried out at the free-electron laser facility FLASH2 at DESY, employing a **pump-probe** approach with UV-excitation and an X-ray probe to track boron-specific electronic changes following excitation.[2]

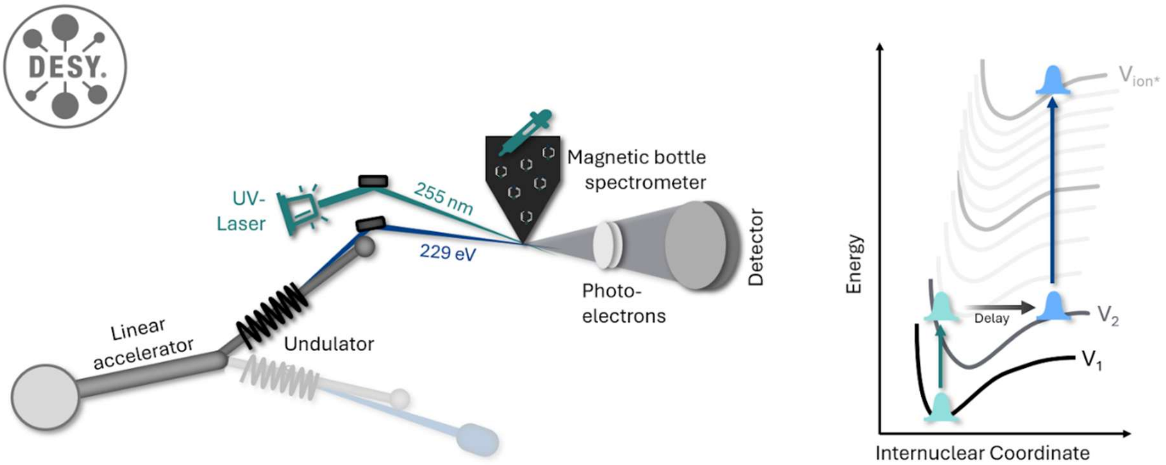

Figure 1: Overview of the experimental setup, alongside the used energy scheme.

Both rapid relaxation through a conical intersection and slower, long-lived dynamical processes were observed. Supported by static **theoretical calculations** and **quantum dynamic simulations**, insights were gained into excitation energies, the formation of long-lived reaction products, and the underlying relaxation pathways.

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13

Catalytic Si/B Exchange Condensation as a Mild and Efficient Route to Conjugated Alkynyl-Spaced Boranes

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Conjugated organoborane compounds have been the subject of enormous research efforts in recent decades due to their versatile applications in materials science, such as in organic photovoltaics (OPVs) or light-emitting diodes (OLEDs).[1] In order to achieve and tune the desired electronic and optical properties, effective overlap of the vacant p_π-orbital of boron with the orbitals of the adjacent π-system is essential. A promising architecture in this context are essentially cyclolinear oligoboranes, in which the boron center is bound to two aromatic rings through which π-conjugation takes place. A third bulky aryl substituent usually provides kinetic stabilization of the boron center.[2] This type of architecture, however, only allows for a limited selection of aromatic systems that enable an effective extension of the π-conjugation across the boron center due to the steric nature of these groups: if they are too large, severe deviation from an ideal coplanar arrangement between their π-systems and the trigonal planar BR_3 plane occurs, mitigating the desired conjugation across the compound’s backbone.

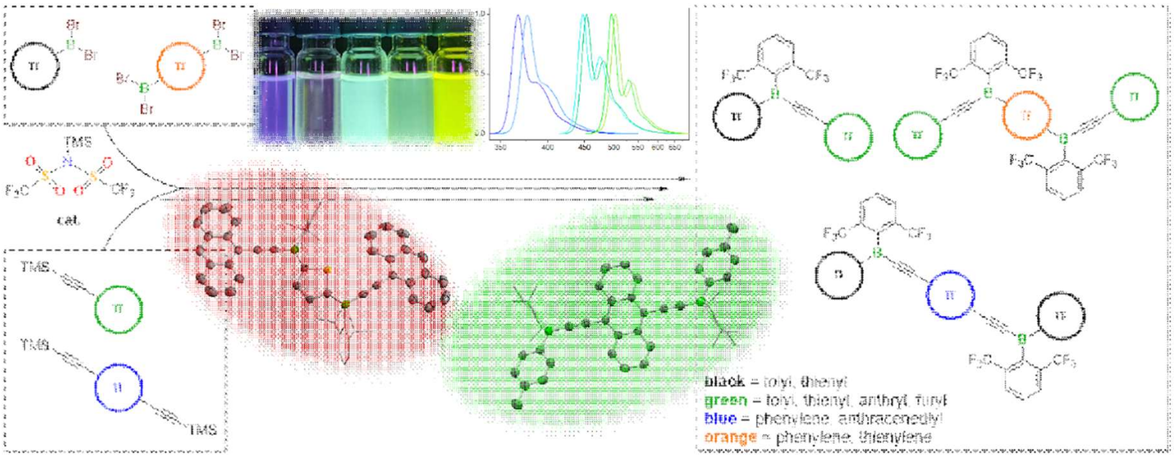

Figure 1: Schematic representation of the synthesis of alkynyl-spaced boranes via catalytic Si/B exchange reaction and examples of their solid-state molecular structures and photophysical properties.

A promising option for overcoming this problem is the insertion of an alkynyl spacer between the boron center and one of the aryl or arylene substituents. We recently succeeded in the synthesis of air and moisture stable alkynyl-spaced boranes and bisboranes by means of a catalytic Si/B exchange reaction. This modular approach enables the variation of both the boron- and alkynyl-bound substituents. The obtained conjugated boranes display a high degree of coplanarity of the central BC_3 plane(s) with both the boron- and alkynyl-bound substituents, allowing effective extended π-conjugation. This is substantiated by single-crystal X-ray diffraction as well as photophysical and electrochemical measurements.[3]

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14

In-vitro selection of ribozymes for fluorescent labeling of RNA that contain epitranscriptomic modifications

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Epitranscriptomic modifications in natural RNA such as 5-methylcytidine and pseudouridine greatly influence RNA structure and function[1]. Studying these modifications' roles in health and disease requires their site-specific detection, which can be achieved via fluorescent labeling. Previously, ribozymes have been used for site-specifically targeting canonical nucleosides in RNA[2], but not yet for labeling of modified RNA. In vitro selection is a powerful tool for discovering new ribozymes.

My research aims at discovering ribozymes through in-vitro selection that catalyze the attachment of a bioorthogonal label to the modified ribonucleotide in a substrate RNA. These ribozymes should preferentially label modified over unmodified ribonucleotides and enable the attachment of fluorophores via click chemistry. The in-vitro selection scheme to discover such ribozymes from a random RNA library was inspired by our previous work on tenofovir-transferase ribozymes[3]. Here, the goal was to find ribozymes that label 5-methylcytidine in an RNA substrate sequence, and other ribozymes that label pseudouridine, but ideally they should be less active on unmodified RNA. Several ribozymes were discovered, and their activity, specificity and possible future applications will be presented. The challenges of finding selective ribozymes through in-vitro selection, methods of overcoming these challenges, and the possible roles of these ribozymes in furthering epitranscriptomic research will be discussed.

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15

Poly(*p*-phenylene phosphaborene): towards Recyclable BP Congeners of Poly(*p*-phenylene vinylene) for Sustainable Electronics

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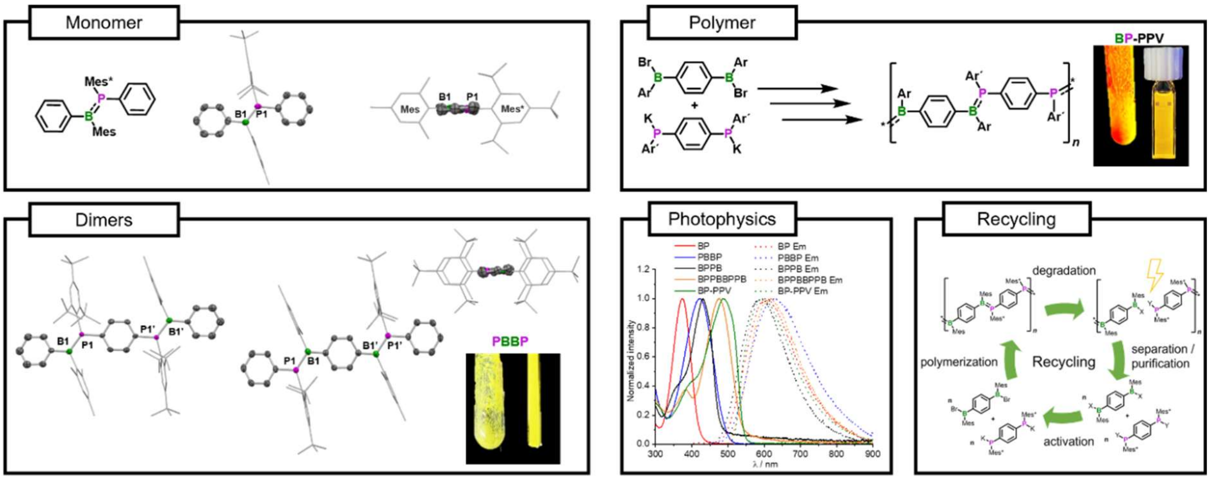
The replacement of selected C=C units in well-established π-conjugated organic materials by isosteric and isoelectronic heteroatomic units, e.g., B=N,[1] has led to various novel hybrid materials, many of which show intriguing properties and functions. Our group recently presented an unprecedented BN-modified poly(*p*-phenylene vinylene) (PPV).[2]

We now aimed at introducing valence isoelectronic B=P units into such PPVs. We prepared the first poly(*p*-phenylene phosphaborene) (BP-PPV) as well as BP-PPV-type oligomers, which exhibit a planar backbone with extended π-conjugation. Our novel BCP compounds show distinct fluorescence emission in solution and low temperature phosphorescence.[3] The introduced B–P bond also serves as a predetermined cleavage point, which could provide the fundament for a full recycling process. So far, we made first achievements towards selective degradation of these compounds.



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16

Poly(ferrocenylene iminoborane), Related Copolymers and Macrocycles

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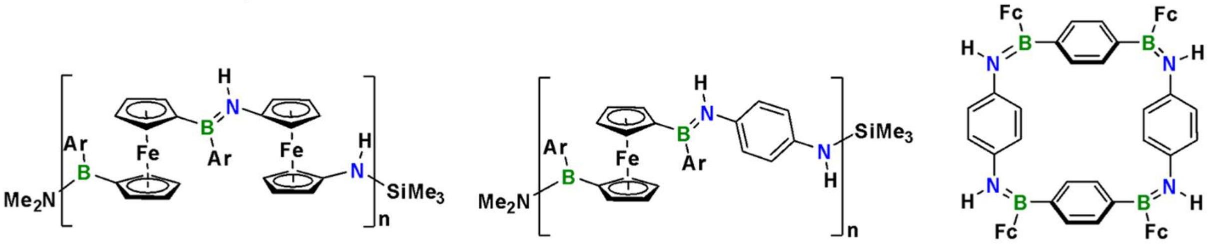
Modification of organic compounds through selective B=N for C=C replacement has developed into a powerful approach to produce new materials with intriguing properties.[1] In recent years, we have presented a number of inorganic–organic hybrid polymers and oligomers that feature B=N linkages in the backbone.[2,3] This includes a BN analogue of poly(*p*-phenylene vinylene) (PPV)[2b,c,j] and inorganic analogues of polyacetylenes, i.e., poly(iminoborane)s.[3] We now present a novel polymer composed of B=N-linked ferrocene units, **1**,[4] and related copolymers with additional *p*-phenylene building blocks **2**.[4,5] Our synthetic approach provides access to a donor–acceptor backbone structure due to the NNBB sequence of the heteroatoms along the chain. Highly valuable insights into the microstructure of the novel metallopolymers as well as into the electronic communication over the π-bond of linear B=N moieties in general are presented. We also explored the incorporation of ferrocenyl groups as side chains into BN-PPV-like structures. This yielded, besides cyclolinear oligomers of that type, the novel macrocycle **3**.[2f]



1 **2** **3**

Figure 1. BN-doped polymers **1** and **2** and macrocycle **3** (Ar = Mes, Tip, Fc).

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Aromaticity in Charged and Neutral Boraporphyrins

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Porphyrins are a naturally abundant class of macrocyclic chromophores that play important roles in natural processes, *e.g.* photosynthesis. Steadily growing research interest has led to a plethora of synthetic porphyrins, some of which have been tailored for specific applications, such as sensitizers in dye-sensitized solar cells (DSSCs) or light-harvesting materials in organic photovoltaic cells (OPVs).[1] Thus, the ability to efficiently modify their opto-electronic properties is crucial. Our group has recently reported on highly luminescent π-conjugated oligofuryl-bridged bis- and polyboranes.[2] Encouraged by these results, we aimed at incorporating the difurylborane moiety into porphyrins to obtain boraporphyrins that are unprecedented in the literature. We successfully synthesized first examples of furan-based expanded diboraporphyrins and their aromatic dianions,[3] as well as 5-bora-21,22-dioxaporphyrin and metal complexes thereof.[4] The boraporphyrins exhibit strong absorption in the visible and infrared spectral range, enhanced photoluminescence, and versatile electrochemical properties. Experimental data suggests significant aromaticity, which we have also investigated by detailed computational studies.

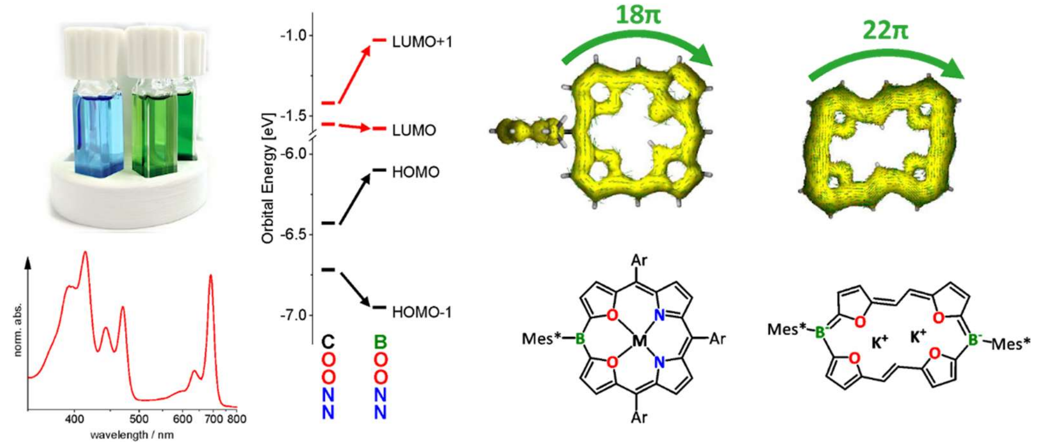

Figure 1: Structures, ACID plots, orbital energies, and absorption spectra of boraporphyrins and diboraporphyrins including their colored solutions.

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18

Visible-Light-Induced Bond Homolysis of Titanacyclopentadienes for the Catalytic Cyclodimerization of Internal Alkynes

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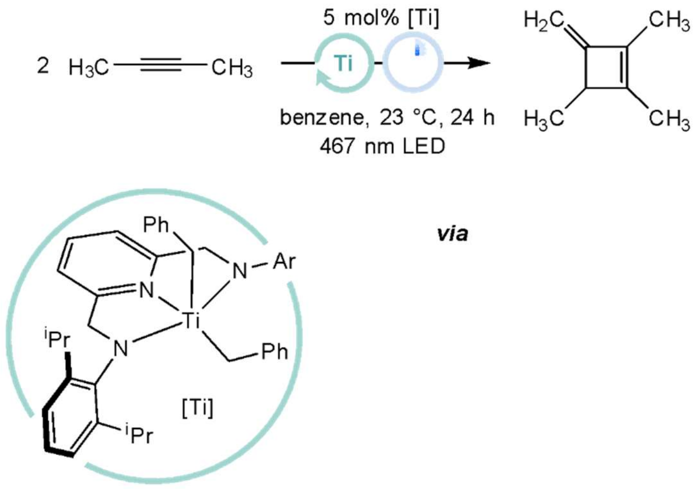
The oligomerization of alkynes is a well-known reaction in organometallic chemistry and provides useful building blocks from readily available chemicals. In the case of titanium, cyclotrimerization of terminal or internal alkynes to arenes is frequently reported.[1] Moreover, the dimerization of terminal alkynes to enynes is a well-precedented reaction.[2]

Using a pyridinediamido titanium dibenzylcomplex,[3] we present the catalytic cyclodimerization reaction of internal alkynes such as 2-butyne to afford methylenecyclobutenes. These molecules are complex building blocks containing an unsaturated four-membered ring, an exocyclic double bond and a new sp^3-hybridized carbon atom. Mechanistic investigations suggest light-accelerated formation of a titanacyclopentadiene, which is also the resting state during the reaction. Kinetic analyses give important insights into the rate-determining steps of the reaction. Additional mechanistic insights were obtained from stoichiometric reactions as well as TD-DFT calculations.



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Titanium-Mediated Multi-Electron Activation and Atom-Transfer Catalysis with Sulfur

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The development of sustainable, efficient and environmentally benign catalysts plays an important role in the future development of synthetic procedures in both academia and industry.[1] Currently, a significant portion of catalysis is reliant on rare and often toxic late transition metals such as palladium, iridium and rhodium.[2] In contrast, titanium is the second most abundant transition metal in earth's crust as well as biocompatible.[3] The high stability of titanium in the oxidation state +IV, however, currently limits its application as a catalyst for redox processes.[4] Utilising redox active ligands can aid in overcoming this limitation through metal-ligand-cooperativity (MLC), allowing for ligand-centred redox reactivity as opposed to the more established metal-centred redox reactivity.[5] To the best of our knowledge, the only example for the implementation of titanium +IV complexes bearing redox active pincer ligands in group-transfer catalysis was reported by *Wolczanski*, who reported the catalytic synthesis of adamantly-isocyanate from the respective organic azide and CO.[8]

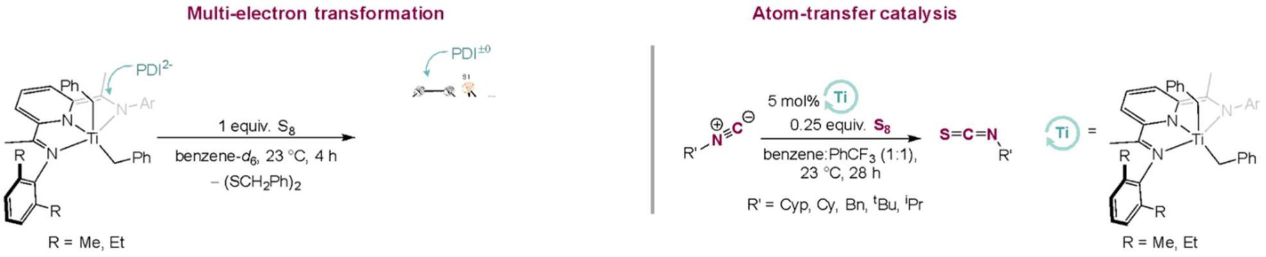

Figure 1: Left: Four-electron activation of sulfur, Right: Sulfur transfer catalysis.

In our work, we present a novel four-electron activation of elemental sulfur with a titanium +IV complex utilizing two electrons generated *via* reductive elimination of bibenzyl in combination with two electrons which are contributed by the redox active ligand diiminopyridine (PDI), , leading to the isolation and characterisation of a rare titanatetrasulfido-spiropentane moiety (Figure 1, left).[9] Leveraging this unique four-electron reactivity enables the implementation of these complexes as highly efficient catalysts for sulfur atom-transfer to isonitriles to selectively form isothiocyanates under mild conditions.

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There and Back Again – the journey of a magnetic transfer between ^{1}H and ^{14}N nuclei under fast MAS.

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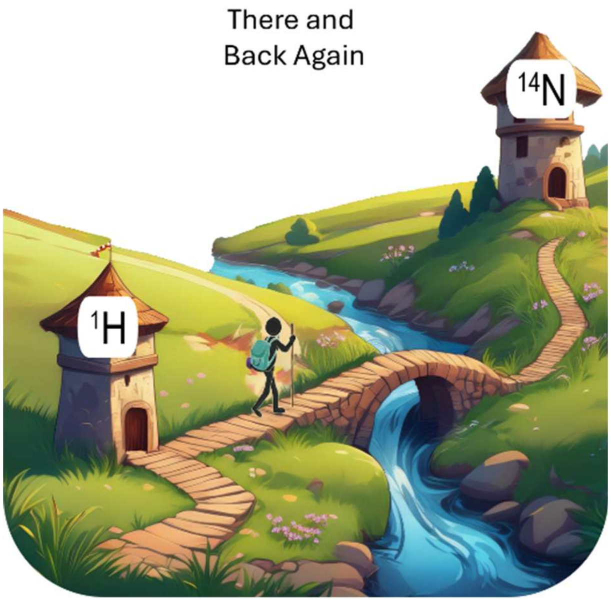

Figure 1: Graphical illustration of magnetic transfer between protons and ^{14}Nitrogen.

NMR spectroscopy using the ^{14}N nucleus has a wide range of applications as nitrogen occurs in many organic, biological or medical systems. Due to its spin of ½, the ^{15}N nucleus is often preferred over the spin-1 nucleus with its quadrupolar interactions, although the natural abundance of 99.64% clearly favours ^{14}N. The challenges of quadrupole interactions and the low gyromagnetic ratio of the nitrogen nucleus can be overcome by using fast MAS and magnetization transfer from ^{1}H to ^{14}N.[1] Hydrogen-nitrogen interactions, particularly those involving intra- or intermolecular hydrogen bonds, can contribute to our understanding of structure and function, clearly worth a closer look.

Two types of ^{1}H-^{14}N correlation experiments were compared: the ^{1}H-^{14}N HMQC (Heteronuclear Multiple Quantum Coherence) experiment and the ^{1}H-^{14}N DCP (Double Cross Polarization) experiment. In the HMQC experiment, two-way magnetization transfer occurs through dipolar recoupling of ^{1}H and ^{14}N nuclei, which generates heteronuclear coherence.[2] In the DCP experiment, the magnetization is transferred from ^{1}H to ^{14}N, and back again using two optimized CP pulses.[3] Both methods can be used to determine direct NH, as well as longer-range ^{1}H-^{14}N correlations.

The two experiments were implemented and thoroughly optimized using crystalline histidine and the dipeptide AspAla. They were then applied to systems with different levels of crystallinity, rigidity, and size, such as the small molecule drug atorvastatin (crystalline as well as amorphous). Based on this set of samples, similarities, differences, and respective advantages and disadvantages will be discussed. For instance, a specially optimized DCP could be tailored to focus on specific ^{1}H-^{14}N correlations, whereas the HMQC would examine all correlations observable at a given recoupling time. Both experiments can be applied to understand structure and hydrogen-bonding patterns in biomolecules and pharmaceutical compounds.

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Analysis of radical-doped polymer micelles for DNP-NMR

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Block copolymer micelles represent a diverse platform for drug delivery systems, potentially including targeting moieties or stimuli-responsive elements to control cargo release.[1] Structural characterization of such complex particles is essential for their development but remains challenging, especially if low-concentration species such as surface groups or active ingredients need to be detected. Solid-state NMR combined with hyperpolarization techniques such as Dynamic Nuclear Polarization (DNP) provides a solution to this problem.[2]

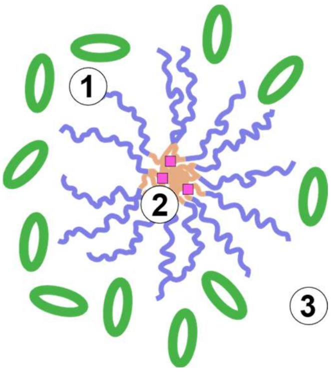

Figure 2: Schematic depiction showing a drug-loaded polymer micelle with numbered sites indicating possible PA deposition at the surface (1), within the core (2), and in the surrounding medium (3).

We are functionalizing polymer end-groups with biradical polarizing agents (PAs) to bring the PAs selectively to specific micellar compartments (Figure 1). Cw EPR spectroscopy enables to probe the radical environment and understand the radical distribution within the micellar aggregates.[3] This lays the foundation for a detailed analysis of the micellar formulation by DNP-NMR. While the DNP-induced signal enhancement occurs throughout the entire sample, depolarization and bleaching effects are restrained to the close vicinity of the PAs.[4] By analyzing these localized signal changes, we can generate spectra that highlight only the molecular components in close proximity to the PAs.

This approach can be used to specifically analyze the drug-rich domain in the micellar core or the excipients outside of the nanoparticles. As a result, detailed information on the spatial arrangement of the molecular components within the micelles and their environment can be obtained.

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Exploring the Potential of BNB- and NBN-doped Phenalenyls: Incorporation into DNA and Donor–Acceptor Oligomers

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Isostructural but electronically distinct chromophores[1] such as BNB- and NBN-doped phenalenyls[2] are an excellent tool for analysing intermolecular interactions with minimal structural perturbation, as well as for constructing novel donor–acceptor PAH frameworks.[3,4]

We introduced an electronically complementary pair of BNB- and NBN-doped phenalenyl-extended nucleosides into deoxyribonucleic acid (DNA), where they act as donor–acceptor pair in a Förster resonance energy transfer (FRET) process.[5] The pair was then applied in a toehold-mediated strand displacement (TMSD) experiment, demonstrating its potential for DNA-based applications (Fig. 1).

Next, we used the complementary building blocks in donor–acceptor dyads and tryads, which exhibit pronounced solvent-dependent charge transfer emission and stimuli-responsive behaviour.[6]

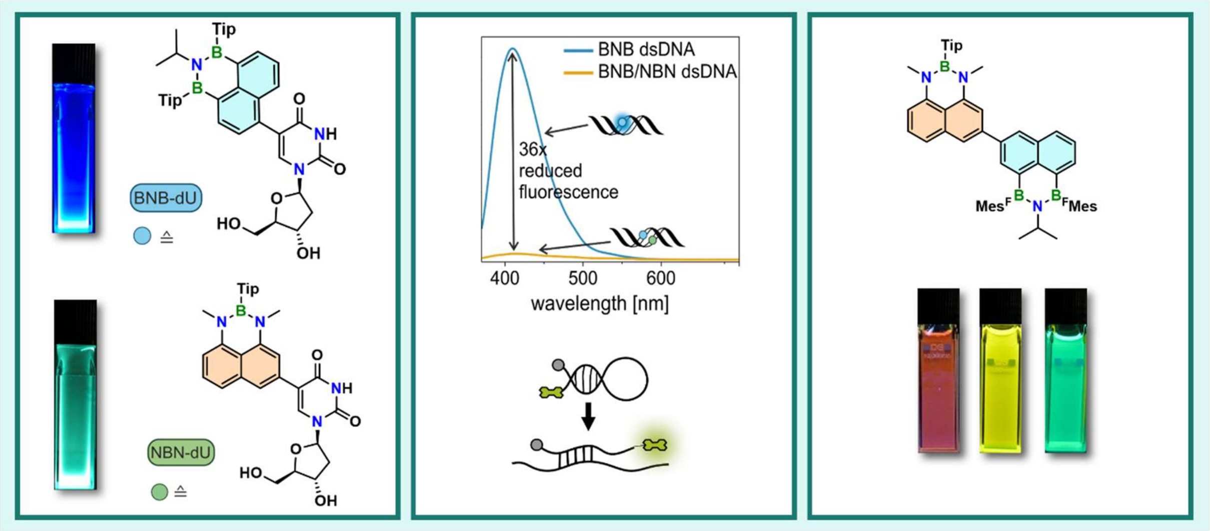

Figure 1: Fluorescent BNB/NBN-doped nucleosides (left), their incorporation into DNA (middle), and donor–acceptor dyads thereof (right).

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Pincer Ligand Transformation at the Metal Center through Hydrogen Atom Abstraction

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Transition metal pincer complexes have emerged as a versatile platform for probing structure-reactivity relationships and enabling diverse catalytic transformations.[1-2] Our group focuses on pincer complexes of the group 4 triad, particularly those featuring redox-innocent pyridinediamido (PDA) and redox-active pyridinediimine (PDI) ligands.[3-4] While these systems exhibit distinct reactivity, interconversion between them traditionally requires a laborius *de novo* synthesis.

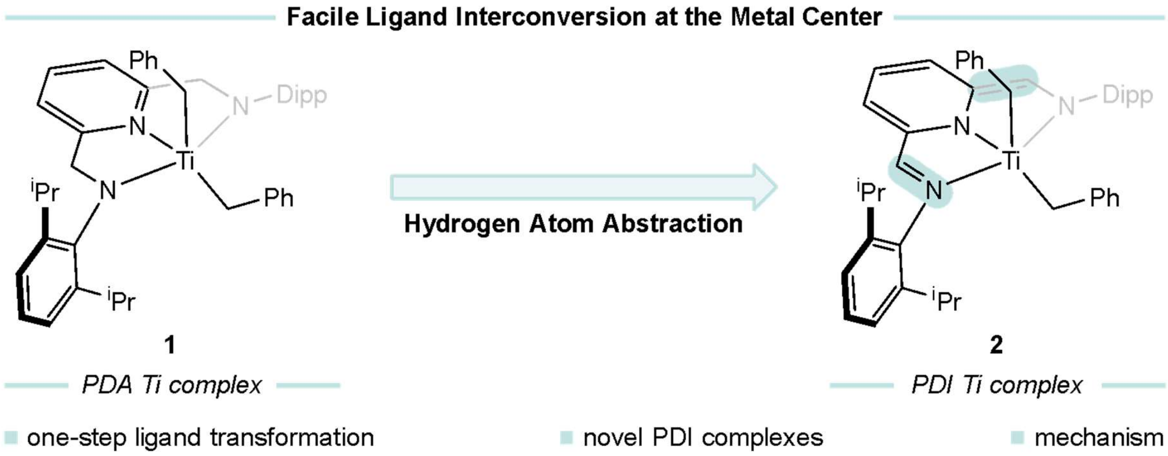

Figure 1: Transformation of a PDA pincer ligand at the metal center to yield the corresponding PDI complex.

In this work, we present a hydrogen atom abstraction reaction of PDA complexes that provides convenient one-step access to the corresponding PDI analogues. As illustrated by the reaction shown in Figure 1, this approach enables selective formation of the target PDI complex **2** in cases where the established coordination-reduction route[5] is compromised by competing overreduction. We systematically probe the applicability of this novel transformation by examining the effect of the metal center, metal-bound substituents, ligand sterics, and choice of the hydrogen atom abstraction reagent. The mechanistic pathway of the hydrogen atom abstraction via proton-coupled electron transfer (PCET) is investigated by measuring a deuterium kinetic isotope effect.

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24

Titanium-Mediated Rearrangement of Bis(alkynyl)boranes: B–C Activation versus C–H Activation

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Tricoordinate organoboranes are important Lewis acids due to the empty *p*-orbital on boron. Bis(alkynyl)boranes feature a tricoordinate boron center substituted with two alkynyl groups, enabling bifunctional reactivity: the boron center engages in TM→B dative bonding, while alkynyl substituents participate in metal coordination. Previous studies in the Ye group confirmed η^5-coordination mode of bis(alkynyl)boranes to zirconium and later uranium, and revealed a uranium-mediated rearrangement delivering uranium-fused boracyclobutenes (zigzag-structure).[1,2] BN-butafulvenes were also obtained, highlighting the unique chemical property enabled by this motif.[3]

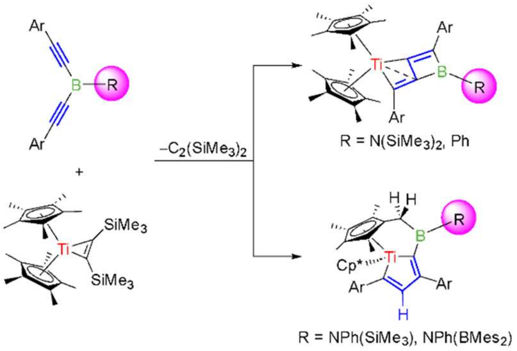

Figure 1: Two Ti-mediated bis(alkynyl)borane rearrangement modes.

In this work, the titanium-mediated rearrangement of bis(alkynyl)boranes to form zigzag-structure was successfully achieved (Figure 1, top).[4] This represents the first realization of this rearrangement within the *d*-block transition metal and overcomes the previous limitation of an amino substituent on boron observed in uranium system. Moreover, employing two new bis(alkynyl)boranes uncovered a novel titanium-mediated rearrangement pathway (Figure 1, bottom). X-ray analysis confirmed the structures, revealing that the two alkynyl groups rearranged to generate a titanacyclopentadiene framework, which is tethered to one of the cyclopentadienyl ligands through a $–CH_2–BR–$ bridge. DFT calculations reveal an unprecedented mechanism involving an initial η^2-coordinated bis(alkynyl)borane intermediate. The subsequent selectivity between B–C activation and C–H activation is governed by boron substituents. When the boron center bears substituents with +M effect (–Ph) or β-effect (two $–SiMe_3$ groups), both efficiently increase of positive charge on boron, thereby favoring B–C activation. In contrast, when compounds lack sufficient silicon β-effect, the C–H activation pathway becomes more dominant instead.

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25

Poly(arylene iminoboranes): a new class of inorganic–organic hybrid polymers with stimuli-responsive behavior

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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.[1,2] We reported the first poly(*p*-phenylene iminoborane), which is derived from poly(*p*-phenylene vinylene) (PPV) by replacement of its vinylene with B=N moieties (i.e., BBNN-PPV).[3]

Next, we targeted a BN/CC isostere of poly(thiophene vinylene) (PTV), namely, a poly(thiophene iminoborane) (BBNN-PTV),[4] as well as mixed copolymers combining both PPV and PTV.[5] The polymers and a series of monodisperse oligomers showed solid-state fluorescence, aggregation-induced emission (AIE) behavior, and pronounced π-conjugation over the B=N units. With the goal of introducing a permanent dipole into the chain, we recently also accomplished the synthesis of a strictly alternating BN-PPV and corresponding monodisperse oligomers. The compounds showed pronounced dual-emission fluorescence behavior and stimuli-responsive properties to water (aggregation emission enhancement; AEE), solvent polarity and viscosity, temperature, as well as mechanical impact.[6,7]

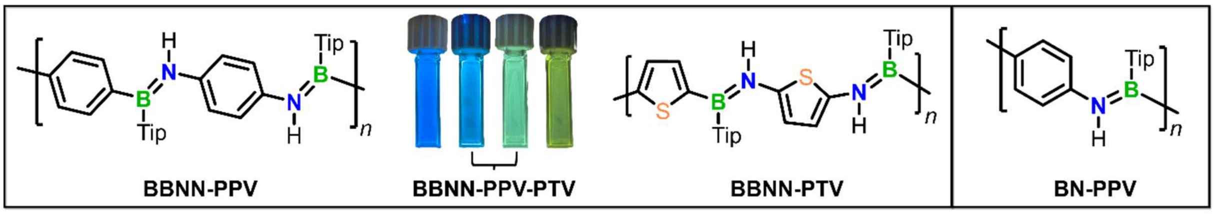

Figure 1: Structures of BBNN-PPV, BBNN-PTV, and their films under UV light, as well as BN-PPV.

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26

Introduction of the Bis(trifluoromethyl)amino Group into Organic Molecules

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The *N,N*-bis(trifluoromethyl)amino group $N(CF_3)_2$ represents a remarkable fluorinated and non-toxic functional motif characterized by high chemical stability and low basicity.[1] However, the synthetic utility of the $N(CF_3)_2$ group has remained limited due to the lack of convenient starting materials and methods for the introduction into organic frameworks.[1] For the former, a breakthrough was achieved with the development of $CF_3SO_2N(CF_3)_2$ and $(CF_3)_2NSO_2N(CF_3)_2$, which can easily be synthesized on a large scale via electrochemical fluorination (Simons process) and enable the generation of the $\{N(CF_3)_2\}^-$ anion by reaction with organic and inorganic fluoride salts.[2] We have successfully established this route and building on this foundation, developed ligand-stabilized transition-metal and alkali-metal salts as suitable and stable transfer reagents.[3] Additionally, we have synthesized $(CF_3)_2NC(O)F$ via electrochemical fluorination as a potential, more efficient carrier of the $N(CF_3)_2$ group.[4]

Furthermore, we have developed new complementary strategies to facilitate the incorporation of the $N(CF_3)_2$ group into organic molecules. In this regard, we recently reported an efficient synthesis of *N,N*-bis(trifluoromethyl)aminoacetonitrile, a versatile building block featuring distinct reactive sites that allow a range of transformations, including Knoevenagel condensations and cyclization reactions towards *N*-heterocycles.[5] In another approach, we investigated the direct reaction of arynes with organic salts of the $\{N(CF_3)_2\}^-$ anion as an efficient synthetic method for the introduction of the $N(CF_3)_2$ group into aromatic systems.[6]

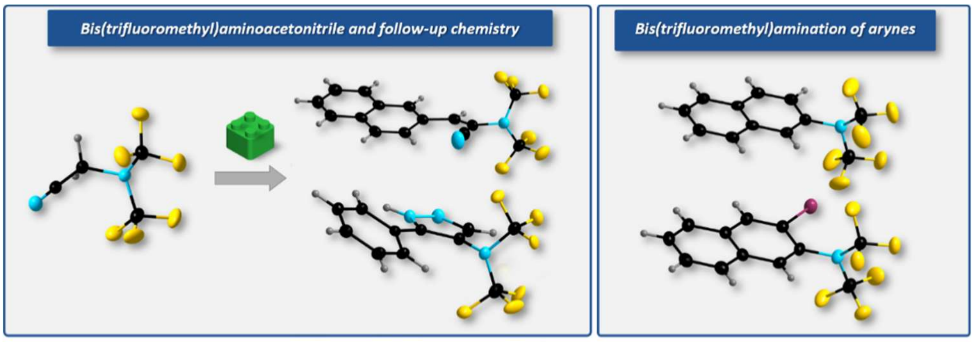

Figure 1: Crystal structures of *N,N*-bis(trifluoromethyl)aminoacetonitrile and representative follow-up chemistry products (left). Crystal structures of *N,N*-bis(trifluoromethyl)amination products of arynes: *N,N*-bis(trifluoromethyl)naphthyl-2-amine and 3-bromo-*N,N*-bis(trifluoromethyl)naphthyl-2-amine (right).[5,6]

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Ab Initio Nonadiabatic Dynamics for Photochemical Processes and Simulation of Time-Resolved Observables

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The investigation of photochemical dynamics requires quantum chemical methods that can accurately describe both ground state and electronically excited states, as well as a framework to enable radiative and nonradiative transitions between them. In our work, we employed the complete active space self-consistent field (CASSCF) method together with second-order perturbation theory (CASPT2) or spin-orbit multireference configuration interaction (CASSCF/SO-MRCI), combined with trajectory surface hopping for the inclusion of nonadiabatic effects to accurately simulate photo-isomerisation of *cis*-stilbene[1] and photochemical dissociation of cyclobutanone[2]. Based on the simulated trajectories, time-resolved observables such as time-resolved photoelectron spectrum (TRPES) or gas-phase ultrafast electron diffraction (GUED) patterns can be predicted.

The *cis*-stilbene molecule was studied using the state-averaged extended multistate CASPT2 method. Our simulation reproduces the experimental time-resolved photoelectron spectrum (*cf.* Figure 1 a–b) and identifies an ultrafast ring closure reaction of *cis*-stilbene, apart from the well-known *cis*–*trans* isomerisation. For the cyclobutanone molecule, which has been studied in the frame of the “Prediction Challenge: Cyclobutanone Photochemistry”, the state-averaged CASSCF/MRCI method was employed. By including spin-orbit coupling and modifying the surface hopping equation to allow intersystem crossing, we demonstrate, contrary to the interpretation of some earlier experimental results, a minimal impact of triplet states on the photodynamics of cyclobutanone excited to its 3s Rydberg state. To enable a direct comparison to future experiments, we simulate the gas phase ultrafast electron diffraction patterns (*cf.* Fig. 2 c–d).

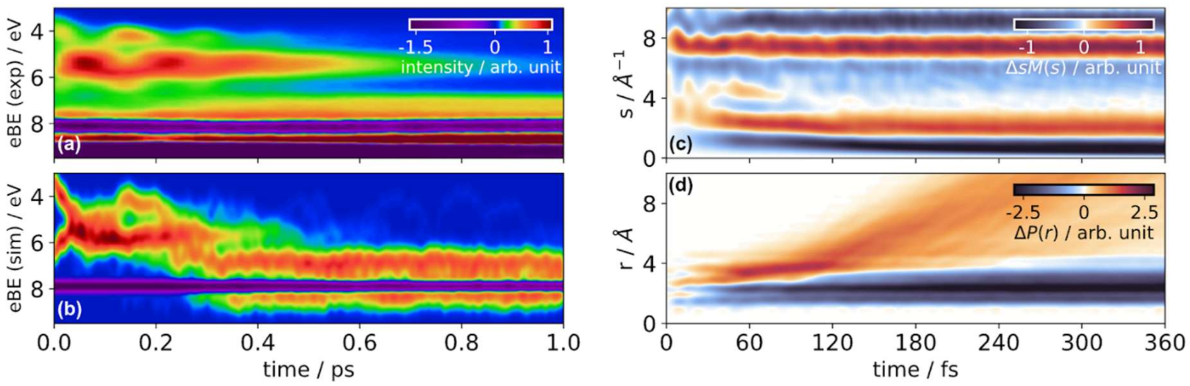

Figure 1: (a) Experimental and (b) simulated time-resolved photoelectron spectrum of cis-stilbene[1], (c) Ultrafast electron diffraction pattern and (d) difference pair distribution function of cyclobutanone[2].

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Vibrations Meet Electrons: Probing Doping Effects in Carbon Nanotubes

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Spectroscopy of molecular vibrations provides a sensitive probe of local structure and bonding and reveals how electronic and vibrational degrees of freedom interact and can be tuned by electronic doping. In our experiments, the utilized doping scheme does not involve chemical substitution but controlled charge transfer that shifts the Fermi level and thereby modifies the coupling between electrons and phonons.

Recently, resonance signals with asymmetric line shapes in doped semiconducting nanotubes (s-SWNTs) have revealed coupling between lattice vibrations and low-energy electronic states [1, 2]. The resulting mid-infrared features bear the hallmarks of so-called Fano (anti-)resonances [3].

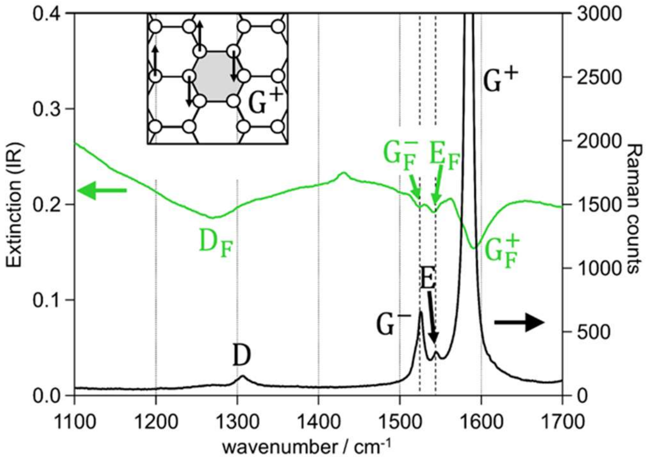

Figure 1: Raman active vibrational modes (black) can be seen in IR spectra after doping (green).

Here, we report the first infrared spectra of doped **metallic** SWNTs alongside doped semiconducting thin films. Distinct resonance signals appear for the Raman-active D- and G-phonons, which gain oscillator strength through coupling to a Drude-like intraband continuum in doped s-SWNTs. Additional fine structure reveals the Raman-active G- and E-modes. In doped s-SWNTs the resonance intensity scales strongly with doping level, whereas in m-SWNTs the dependence is very weak.

These findings establish Fano resonances as a general spectroscopic signature of charge-induced electron–phonon coupling in carbon nanotubes and provide a framework for understanding similar effects in other low-dimensional materials.

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Boron- and Phosphorus-Doped Tetrathiaporphyrinoids

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Macrocycles based on the structural motif of porphyrin play a key role in many essential processes in living organisms such as the binding and transport of O_2 and the conversion of light into usable energy.[1] Lewis acidic π-conjugated organoborane macrocycles on the other hand are currently attracting considerable attention due to their great potential for optoelectronic and sensory applications.[2,3] Incorporation of trivalent boron and phosphorus atoms into the macrocyclic porphyrin framework to customize its electronic structure, however, has only been scarcely studied.

We now succeeded in the synthesis of a porphyrinogen with boron atoms in all four *meso*-positions. Chemical or electrochemical reduction leads to a dianion that features 18 macrocyclic-conjugated π-electrons, thus rendering it a fully aromatic species.[4] Complementary, in order to provide the macrocyclic system with the required number of electrons to fulfil Hückel's rule of aromaticity, a derivative with phosphorus occupying one of the *meso*-positions was conceived (Figure 1). The molecular structure, electronic properties and complexation behaviour of these novel compounds were investigated using X-ray diffraction analysis and quantum chemical calculations.

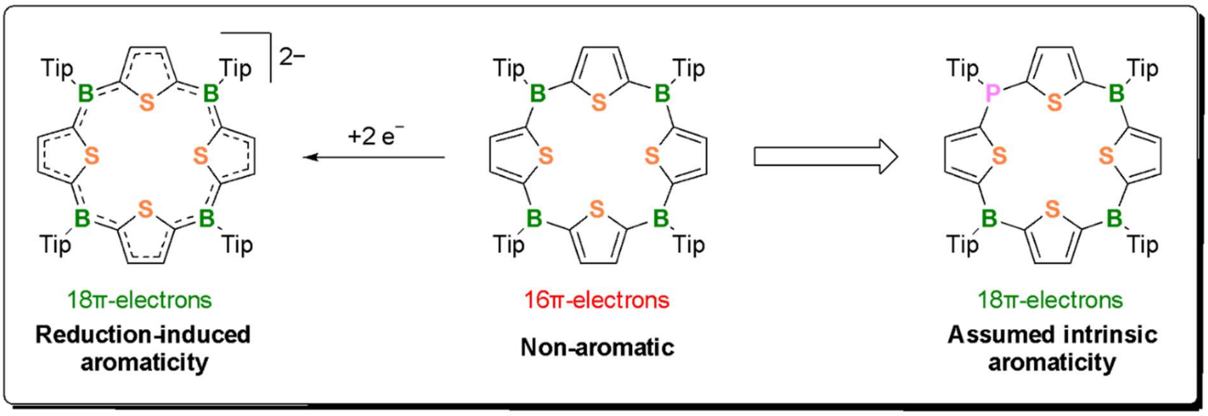

Figure 1: Tetrathiaporphyrinoids and their formal π-electron count (red: non-aromatic; green: aromatic).

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30

Merging Pyrrole with Boron: p-π*-Conjugated Di-(2-pyrryl)boranes

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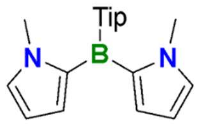
ABSTRACT

During the last decades, π-conjugated materials in which electron-rich organic building blocks are combined with electron-deficient borane moieties have received tremendous attention due to their applications in organic optoelectronics, sensors, and bioimaging.[1,2] Thiophene derivatives have been extensively studied in recent years in this regard.[3-5] Our group has also introduced furan units into boron-doped conjugated materials, which in combination with our Si/B exchange protocol enabled a sustainable approach to strongly luminescent hybrid materials.[3,6,7] Pyrrole congeners thereof, on the other hand, have scarcely been studied.

We developed a multigram scale synthesis of a dipyrryl(tri-*iso*-propylphenyl)borane with methyl groups on the nitrogen atom (**1**) as well as an unprotected derivative (**2**). The structures of both compounds were determined by single-crystal X-ray diffraction, revealing an almost planar structure of the dipyrrylborane unit in **2** and only a slightly twisted one for **1**. The new compounds are intense blue-light emitters due to a TICT character of the excited state structure, as confirmed by TD-DFT calculations. We also investigated the formation of a transition metal complex (**3**) and further extended π-systems such as **4**.[8]



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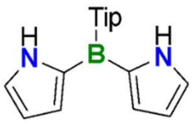

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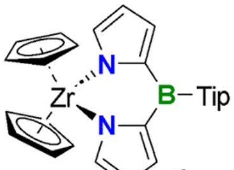

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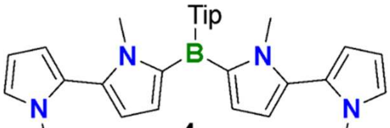

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Harnessing Cooperative Energy Transfer and Hydrogen Atom Transfer for Direct Nitrogenations of non-activated Alkanes

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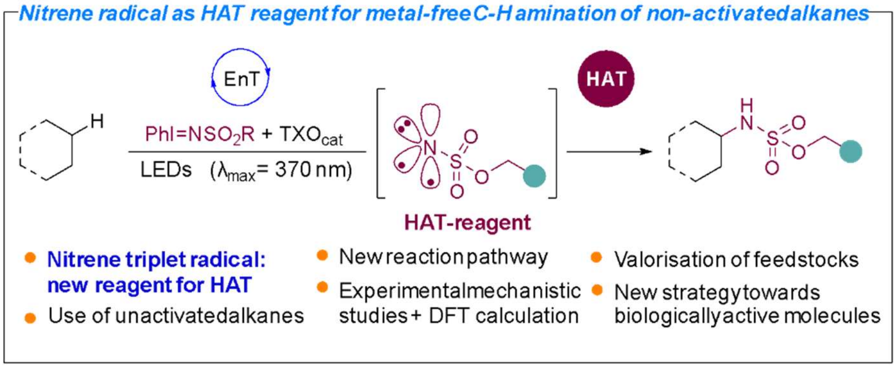
Abstract: While important progress has been achieved recently on direct functionalization of alkanes *via* photocatalytic methods[1,2], direct amination of aliphatic compounds remains a great challenge[3]. Herein we report a conceptually new strategy towards direct conversion of hydrocarbons into amines, based on *in situ* generation of nitrene radical. Energy transfer between thioxanthone (TXO) photocatalyst and iminoiodinane furnishes the triplet nitrene radical, able to undergo HAT reaction promoting alkane activation and subsequent C-N bond formation step. The user-friendly nature of the metal-free transformations, along with mild reaction conditions further highlight the sustainability of this scalable process delivering a diversity of cycloalkylamines.



This photocatalytic reaction occurs smoothly in the presence of TXO photosensitizer and is particularly suitable to convert simple hydrocarbons into valuable amines. Detailed mechanistic studies demonstrate the unusual activation of iminoiodinanes *via* cooperative Energy Transfer / HAT mechanism, the key towards the desired reactivity[4].

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Ultrafast Reflection Spectroscopy of Two-Dimensional Hybrid Perovskites

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Two-dimensional hybrid perovskites have emerged as promising materials for next-generation opto-electronic devices. They consist of alternating inorganic lead-halide layers and long chain organic cations. This Layered arrangement forms a natural quantum well structure which leads to the formation of strongly bound excitons confined within the inorganic layers.[1] By tailoring their chemical composition, key properties such as band gap, exciton binding energy and photoluminescence can be adjusted for specific applications. This makes them potential candidates for use in light emitting diodes or solar cells.[2]

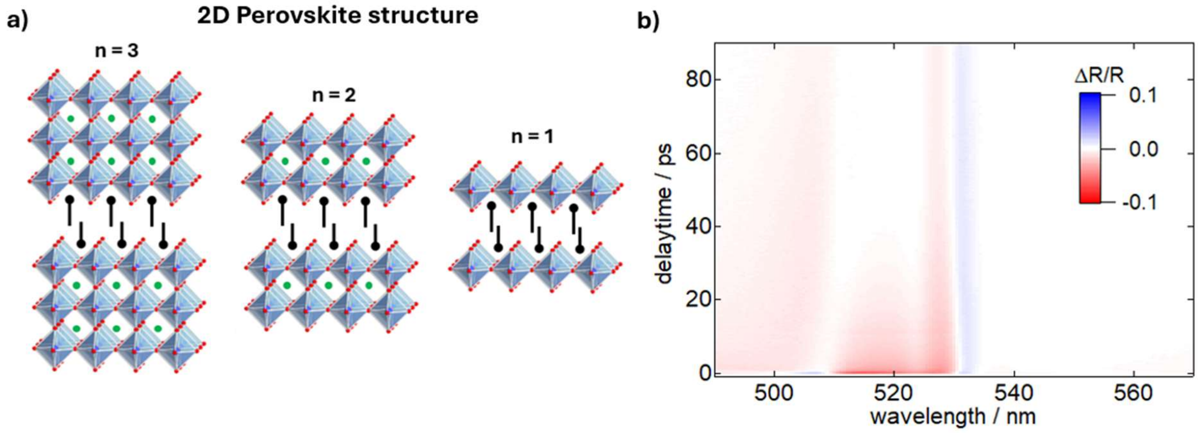

Figure 1: a) General structure of 2D hybrid perovskites in Ruddlesden-Popper phases with decreasing lead-halide layer thickness. b) Time-resolved reflection spectrum of a perovskite sample with the composition PEA$_2$PbI$_4$ (n = 1).

To better understand these materials, we study how excited charge carriers behave after optical excitation. Time-resolved reflection spectroscopy provides a direct way to analyse ultrafast relaxation pathways by monitoring changes in its refractive index.[3]

For this project, a setup for time-resolved reflectance measurements was designed and integrated into an existing laser system. It also includes a microscope to localise the samples and position them in the focal point of the laser pulses. Using this setup, we obtained first time-resolved reflection spectra of a so called stop-band in two-dimensional hybrid perovskites, as shown in Fig. 1. These measurements establish a foundation for future studies of energy transfer and relaxation processes in layered perovskite systems.

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Exploring New Frontiers: Heteroatom-Doped Conjugated Macrocycles, Polycyclic Aromatics, and Inorganic–Organic Hybrid Polymers

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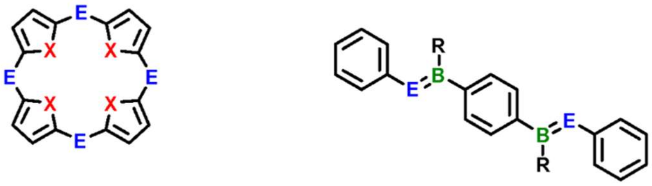
The targeted design of novel π-conjugated materials is of great interest in view of optimizing their performance for various applications such as organic optoelectronics or biomedicine.[1] A promising approach to further diversify the portfolio of π-conjugated molecules and polymers is the incorporation of heteroatoms with a vacant p-orbital, such as boron, or with a free electron pair in a p-orbital, such as nitrogen or phosphorus.



I

X = S, O
E = B-R, N-R, P-R
(R = H, aryl)

II

E = N-R, P-R
(R = H, aryl)

III

E = N-R, P-R
(R = H, aryl)

Figure 1: Heteroatom-doped macrocycles **I** and linear oligomers **II** and **III**.

This computational work focuses on π-conjugated macrocycles, polycyclic aromatics, and conjugated polymers. Selected variants of the frameworks shown in Figure 1 have already been synthesised and characterised by our group. We have recently reported a series of unprecedented boron-doped porphyrinoids.[2] Herein, we present predicted photophysical properties and aromaticity of the porphyrin-based macrocycles of type **I** – including those containing phosphorus in the E-position – using computer-aided quantum chemical methods. In addition, we have investigated the effect of nitrogen and phosphorus substitution in compounds **II** and **III** on their photophysical properties. These cyclolinear conjugated oligomers serve as molecular model systems for heteroatom-doped analogues of poly(*p*-phenylene vinylene) (PPV) and related semiconducting organic polymers.[3]

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Time-Resolved Spectroscopy of Doped Single-Wall Carbon Nanotubes

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The doping of low-dimensional semiconductors and the precise quantification of doping levels remains a major challenge in developing next-generation semiconductor technologies. Semiconducting single-wall carbon nanotubes (s-SWNTs) are one-dimensional cylinders made of a single sheet of carbon atoms and represent one of the most fascinating semiconductor nanomaterials known today. Their optical and electronic properties are dominated by excitons, tightly bound electron-hole pairs. [1-3] Measuring the size of these quasiparticles and how it is affected, for example by doping, is essential for improving our understanding of the photophysical properties of low-dimensional semiconductors and for advancing their potential use in nanoscale optoelectronic devices. [4]

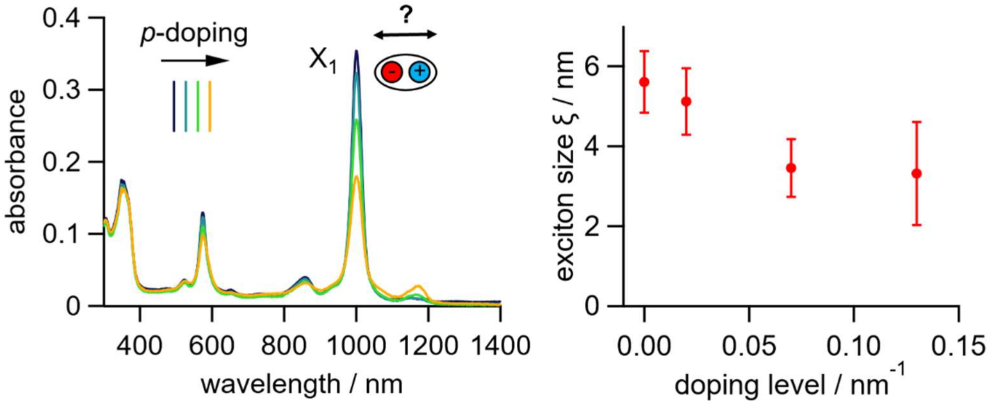

Figure 1: Absorption spectra of *p*-doped SWNTs and the corresponding exciton size..

In this work, we employ femtosecond time-resolved pump-probe spectroscopy to study how excitons behave in doped s-SWNTs. Our measurements on thin films of polymer-wrapped (6,5)-SWNTs provide insights into how doping affects the exciton size and the underlying ultrafast dynamics, revealing a decrease in exciton size with increasing doping level.

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Intra- and Interlayer Excitonic Finestructure of the Two-Dimensional Perovskite PEA_2PbI_4

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Two-dimensional (2D) halide perovskites are organic-inorganic materials with robust stability whose photophysics are governed by quantum and dielectric confinement, resulting in highly tunable excitonic properties.[1–3] However, the absorption and photoluminescence spectra of these materials display several distinct features whose origin is the subject of ongoing debate.[4–6] Here, we study the excitonic fine structure of mechanically exfoliated PEA_2PbI_4 single crystals, combining temperature-dependent photoluminescence (PL) measurements and first-principles calculations using the *GW* and Bethe-Salpeter Equation (BSE) approaches. Our polarization-dependent data confirm the excitonic nature of these features and demonstrate that their fine structure arises from a combination of crystal symmetry and exchange, spin-orbit, and interlayer interactions. Furthermore, we distinguish intra- and interlayer excitons in the spectra and quantify their dipole transition moments. Our findings offer a deeper insight into the rich exciton fine structure of 2D perovskites, advancing our understanding of their photophysical properties.

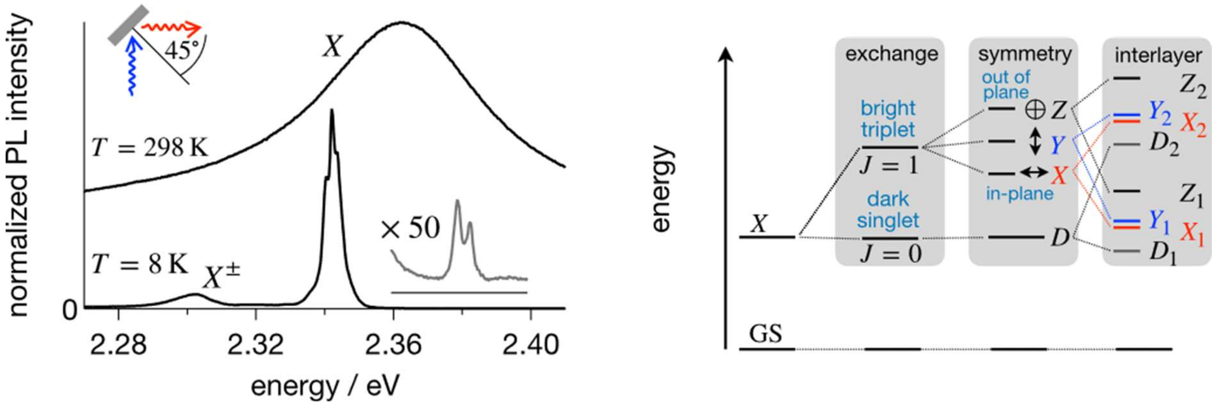

Figure 1: Exciton fine structure of the 2D perovskite PEA_2PbI_4. Normalized PL spectra of mechanically exfoliated PEA_2PbI_4 flakes at room temperature and 8 K (left), and schematic representation of the hierarchy of the excitonic fine structure (right).

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Intermolecular Nickel-Catalyzed C(sp^3)-H Activation

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In the process of creating greener and more sustainable pathways to complex organic molecules, exchanging palladium with its 3d brother nickel in cross-coupling reactions is currently playing one of the leading roles in research. The high reactivity and sustainability of nickel, which is approximately 2,000 times less expensive and 10^4 times more abundant than palladium, make it a highly appealing catalyst for developing sustainable C-H functionalization routes. Recently we have reported the first example of an intermolecular, enantioselective, Ni(II)-catalyzed C(sp^3)–H arylation, providing direct access to challenging all-carbon quaternary stereogenic centers.[1] Key to this success is the use of a specially designed BINOL-derived ligand, which enables efficient desymmetrization of gem-dimethyl groups through a rate- and enantio-determining C–H activation step. This catalytic system demonstrates remarkable functional group tolerance, affording a wide variety of arylated products in high yields (up to 85%) and with good enantioselectivities (up to 95:5 e.r.).

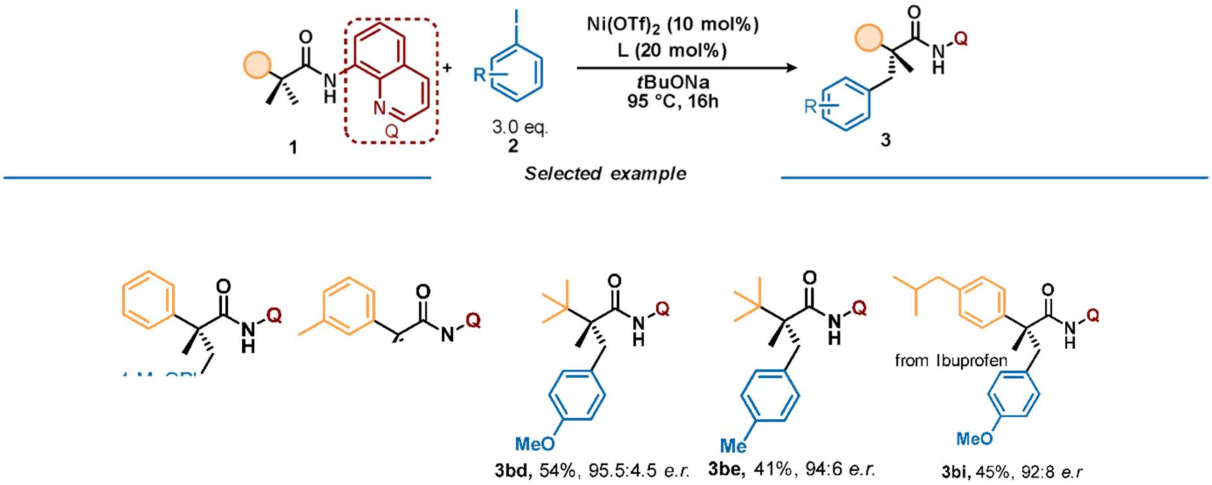

Figure 1: Intermolecular Nickel-Catalyzed C(sp^3-H) Activation.

Even more transformations are enabled by a powerful combination of an aminoquinoline directing group with a Ni (II) catalyst, which is the research our group is currently focused on. A beta-hydride elimination reaction and the arylation of a cyclopropane moiety are opening a wide synthetical window with potential applications in agrochemical and pharmaceutical synthesis.

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DNA-encoded chemistry in organic solvents

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DNA-encoded libraries (DEL) are a technology first invented by Brenner and Lerner in 1992[1] and is now widely used as a screening technology. So far, three clinical candidates resulting from DEL screens have been published.[2-4] However, there are also limitations to DEL synthesis. For example, one major challenge to the translation of synthesis methods to DNA-tagged substrates is the lack of solubility of the highly charged DNA oligomer in most organic solvents. To mitigate that challenge, we discovered the interactions between a neutral poly(*N*,*N*-dimethylacrylamide)–poly(*n*-butyl acrylate) block copolymer, devoid of any canonical DNA-binding structure, DNA oligonucleotides and selective ammonium salts. Due to that interaction, DNA oligomers of up to 80 nucleotides length were solubilized in pure dichloromethane, chloroform, toluene, and in several non-aqueous co-solvents, shown with the help of FAM-labelled DNA oligomers. These ternary DNA–copolymer–ammonium salt interactions led to the formation of aggregates in organic solvents whose size correlated with DNA oligomer length, confirmed by DLS, NMR and TEM measurements.

Figure 1: Cover Art: Aggregation of neutral copolymer with ammonium salt of DNA in organic solvents and its application in IMCR chemistry.

Therefore, this method opened the chemical space for DEL synthesis. This novel approach for DNA solubilization was successfully applied to diversify DNA-tagged starting materials by three isocyanide multicomponent reactions (IMCR), the Ugi, Ugi-azide and Groebke-Blackburn-Bienaymé reactions, with broad scope and excellent yields. The broad scope and excellent yields of these IMCRs should allow for the synthesis of a DEL based on one of these three reactions. Importantly, the copolymer system did not interfere with subsequent DEL operations such as enzymatic DNA tag ligation and barcode amplification. One major advantage of this approach is that the copolymer does not require tailored DNA conjugates, which means it is likely compatible with different DNA-barcoding strategies. As a result, it will likely broaden the toolbox of DEL-compatible synthesis methods well beyond IMCR chemistry.[5]

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Layered Hybrid Materials with Highly Conjugated Guests

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Layered vanadium oxide (V_xO_y) cathodes are promising for multivalent batteries due to their high theoretical capacity and V_xO_y's structural stability. Their practical use remains limited due to V_xO_y dissolution, poor ion diffusion kinetics, and poor electronic conductivity.[1] Strategies such as the intercalation of small molecules or conductive polymers into the VAN-DER-WAALS bonded layers of V_xO_y have shown to enhance the electrochemical performance of V_xO_y cathodes.[2] The performance enhancement observed with small molecule intercalation is mainly attributed to structural expansion of V_xO_y layers via a pillaring effect providing diffusion channels for charge carriers, while polymer intercalation improves electronic transport and suppresses active material leaching.[2] In this work, we aim to combine the pillaring capability of small molecules with the stability of polymers by introducing highly conjugated organic pigment pillars between V_xO_y layers. The pigments are based on rigid, platelet-like perinones (Figure 1**A**), which are electrochemically active, chemically stable, and practically only soluble in H_2SO_4 or hot polar aprotic solvents such as NMP or DMF. These features make perinones ideally suited for improving the performance of layered V_xO_y cathodes. Yet, the poor solubility of perinones renders conventional wet-chemical synthesis routes unsuitable. Recently, we developed a solvothermal route to incorporate perinones into layered titania structures.[3] Based on this route, we developed a synthesis approach in which perinones are synthesized and intercalated into V_xO_y layers in a one-step hydrothermal process starting from aromatic dianhydrides, aromatic diamines, and a V_xO_y source (Figure 1**B**). Analyses reveal that the amount of incorporated perinone governs the resulting structure: Low loadings yield fine, sheet-like structures in a pillared configuration (Figure 1**C**), whereas higher concentrations lead to increasing amounts of perinone–perinone interactions and denser, disordered, presumably turbostratically stacked organic phases within V_xO_y layers (Figure 1**D**).

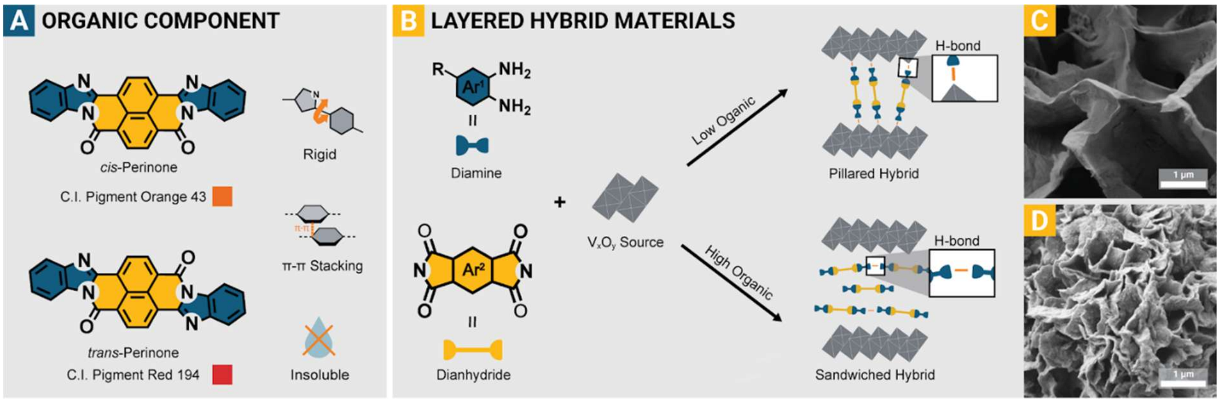

Figure 1: *Cis*- and *trans* isomers of perinone with typical structural and chemical features (**A**). Schematic of the hydrothermal synthesis of perinone VO hybrids with varying organic content (**B**). Scanning electron microscopy images of a pillared hybrid with low organic content (**C**), and a sandwiched hybrid with high organic content (**D**).

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Hydrothermal Synthesis from Renewable Feedstocks

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Green Chemistry focuses on the design of chemical reactions and materials that minimize environmental impact by developing safer, more efficient, and sustainable processes. Two key principles are the use of renewable feedstocks and alternative, greener reaction media.[1]

While compounds derived from natural and renewable resources offer attractive alternatives to petrochemical feedstocks, their share in organic chemical production has remained at around only 9% (2014-2021).[2] This limited proportion may partially be attributed to the fact that only abundant and easily isolable substrates are economically viable. Phenolic compounds, widely distributed in plants, are promising candidates as renewable feedstocks as they can be extracted directly from natural resources or obtained by converting waste from agro-based industries.[3] Phenols are important reagents for the synthesis of benzoxazines, which are precursors for high-performance polymers. However, most benzoxazines are derived from petrochemical reagents such as bisphenols and aromatic amines. Due to the environmental impacts caused by petroleum-based materials, the production of benzoxazines from renewable phenols is gaining attention as a route to sustainable, bio-based polymers.[5] Traditionally, benzoxazines are synthesized in toxic organic solvents such as dioxane or chloroform.[6] Water, in contrast, is abundant, non-toxic, and environmentally benign. Under hydrothermal (HT) conditions – above its atmospheric boiling point and at autogenous pressure – water's physicochemical properties can be tuned to meet specific reaction requirements.[7]

This study explores the combination of renewable phenolic feedstocks with water as a green solvent for the HT synthesis of bio-based benzoxazines. The environmental impact of the approach will be compared to conventional methods by applying green chemistry metrics such as atom efficiency, E-factor, or life-cycle assessment approaches.[1] Overall, this work aims to demonstrate how solvent choice, feedstock selection, and reaction design can be integrated to create a sustainable reaction system.

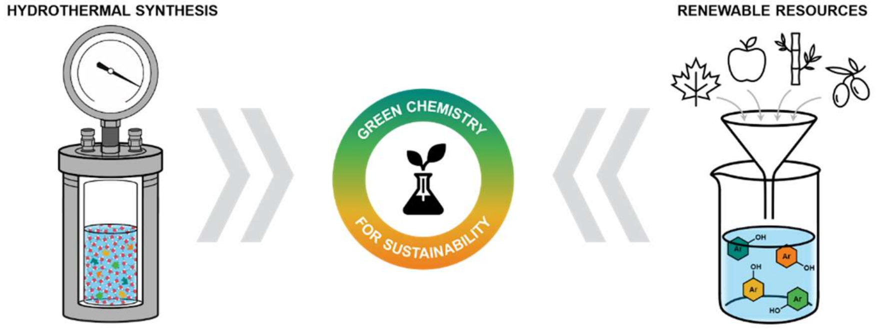

Figure 1: Aspects of sustainable reaction design to obtain apply green chemistry.

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Polyimide-intercalated MnO_2 for battery applications

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Manganese dioxide (MnO_2) is one of the most promising candidates as cathode material for aqueous zinc-ion batteries (AZIBs) due to its natural abundance, multiple stable manganese valence states(Mn^{2+}, Mn^{3+}, Mn^{4+}, Mn^{7+}), and high theoretical capacities of 308 and 616 $mAh\cdot g^{-1}$ for the Mn^{4+}/Mn^{3+} and Mn^{4+}/Mn^{2+} redox reaction, respectively.[1] However, MnO_2-based cathodes in AZIBs often suffer from performance degradation caused by Mn^{2+} dissolution or irreversible phase transformation induced by reactions with Zn^{2+} or H^+. Among the various MnO_2 polymorphs, layered MnO_2 (birnessite) is particularly attractive because of its open interlayer spaces, enabling facile chemical modification and intercalation. To address the aforementioned challenges, conductive polymers like polyaniline and polypyrrole, as well as small organic molecules can be intercalated into the MnO_2 layers to enlarge the interlayer spacing, which facilitates ion transport and improves the stability of the layers. However, the incorporation of such conductive polymers or small molecules can introduce new issues, including poor cycling stability arising from polymer degradation or the dissolution of the organic components into the electrolyte.[2] To circumvent these problems, we aim to intercalate polyimides (PIs) into the layered framework. PIs are known for their excellent thermal and mechanical stability as well as their insolubility in common solvents. Additionally, as they feature imide groups, they not only offer a stable host for metal ions but can also undergo reversible redox reactions which can be beneficial for cycling performance.

Recently, our group showed that those materials can be conveniently synthesized in water or alcohols starting from a dianhydride and a diamine, or from their corresponding monomer salt (MS) which can be readily obtained from the pristine monomers. Those MSs are attractive since they possess ideal 1:1 stoichiometry and high oxidative stability – essential when working with oxidizing materials like MnO_2 – as well as ammonium groups that are highly beneficial for successful intercalation reactions. Furthermore, our group was able to convert the MS into the final PI by solid-state polycondensation,[3] which is also advantageous given the instability of layered MnO_2 in water or alcohols at elevated temperatures.

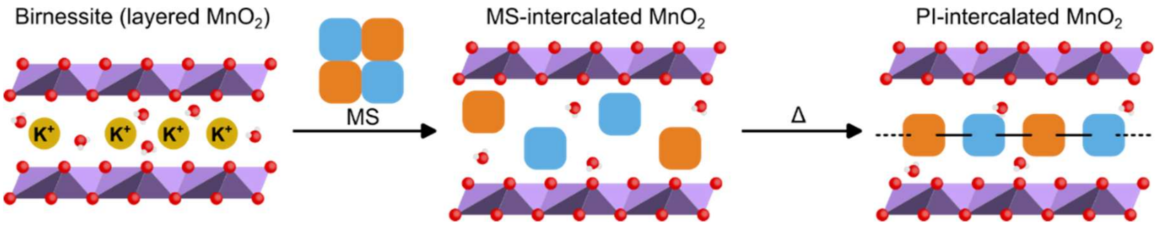

Figure 1: Schematic representation of the polyimide-intercalated MnO_2 hybrid material synthesis, orange and blue rounded squares describe the individual monomers, MnO_2 layers are shown in purple. The pristine MnO_2 is first intercalated with a monomer salt (MS) which can then be transformed upon thermal treatment to the PI-intercalated MnO_2.

Herein, we present a new strategy to intercalate PIs into layered MnO_2 to form confined organic–inorganic hybrid materials (HMs). The synthesis process, schematically depicted in Figure 1, involves the intercalation of birnessite-type MnO_2 with an MS to yield an MS-MnO_2 intermediate, which is subsequently transformed into the desired PI-MnO_2 hybrid by thermal treatment. We believe that our approach yields materials that may suppress Mn dissolution, stabilize the layered framework, enhance ion transport through increased interlayer spacing, and provide robust hosts for metal ions. We present our recent advances on these HMs, which show promising characteristics as cathodes for aqueous Zn-ion batteries.

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Ultrafast Excited-state Dynamics of 4-Hydroxychalcone: Role of Intramolecular Charge Transfer and Photoacidity

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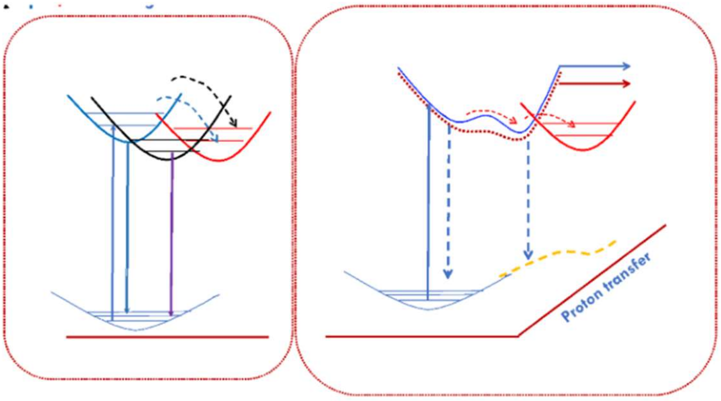

Scheme: Schematic representation of the excited-state dynamics of 4-HC and 4-HC:MI/TBA adducts upon photoexcitation.

Diarylketones such as benzophenones, oxybenzones, chalcones and their derivatives exhibit promising applications as UV filters/sunscreen agents due to their effective absorption in the UV region and dissipation through non-radiative pathways.[1,2] However, elucidation of underlying photoreactive mechanism is non-trivial due to the ultrafast lifetimes of transient species, involvement of non-adiabatic curve crossings among the potential surfaces, etc. In this context, we investigate the excited-state photoreaction dynamics of 4-hydroxychalcone (4-HC) under various environments through femtosecond–transient absorption (fs–TA), nanosecond–transient absorption (ns–TA), and femtosecond–fluorescence upconversion (fs–FL) measurements. Steady-state fluorescence measurements of 4-HC in presence of 1-methylimidazole (MI)/tert-butylamine (TBA) exhibit dual band emission. The fs-TA measurements of 4-HC in presence of MI/TBA exhibit distinct spectral and associated lifetimes as compared to 4-HC alone indicating a significant interaction of the hydroxyl proton with bases and influencing the reaction dynamics. The 4-HC:MI/TBA adduct undergoes excited-state intermolecular proton transfer within a time scale of ~500 fs and subsequently relaxes back to the ground state through long–lived triplet state. The experimental observations of excited–state reaction dynamics of 4–HC in presence of MI/TBA bases have been well corroborated with the computational analysis.

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Boron- and Phosphorus-Based Weakly Coordinating Anions

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Weakly Coordinating Anions (WCAs) are characterized by their exceedingly weak interactions with cations and high chemical robustness. Thus, WCAs enable the stabilization and often isolation of highly reactive, electrophilic cations that otherwise cannot be handled.[1] For example, they find application as inert counterions in cationic catalysis. In the field of electrochemistry, fluorinated WCAs are important compounds for electrolytes in metal-(lithium-)ion batteries and supercapacitors. In summary, WCAs are indispensable building blocks for modern synthetic and applied chemistry.[2]

In recent years, our research group studied different types of weakly coordinating phosphorus- and boron-anions. An important class of compounds are pentafluoroethyl(fluoro)phosphate anions $[(C_2F_5)_nPF_{6-n}]^-$ (n = 1–3), which were applied as electrolyte components in metal-ion batteries. More recently, the $[(C_2F_5)_3PF_3]^-$ anion (FAP[3]) was used for the stabilization of transition metal complexes for applications in catalysis.[3] The hexacyanodiborane(6) dianion decorated with six tris(pentafluorophenyl)borane units represents an unusual WCA that for example, is capable in stabilizing the highly reactive $\{H(OEt_2)_2\}^+$ cation. The so far weakest coordinating anion is the tetrakis(trifluoromethyl)borate anion $[B(CF_3)_4]^-$, first synthesized by Willner *et al.*[4,5] Since it is well known that the coordination ability is inversely related to the anion volume (anions of same charge), we started to investigate perfluoralkylborate anions with longer alkyl chains. Two first representatives, $[(C_2F_5)B(CF_3)_3]^-$ and $[(C_2F_5)_2B(CF_3)_2]^-$ were recently synthesized in our group that indeed are even less coordinating than the $[B(CF_3)_4]^-$ anion. Perhalogenated anionic boron clusters such as $[1\text{-}H_2N\text{-}\textit{closo}\text{-}1\text{-}CB_{11}Hal_{11}]^-$ (Hal = F, Cl) are another class of WCAs that are of interest for materials chemistry and medicinal applications.

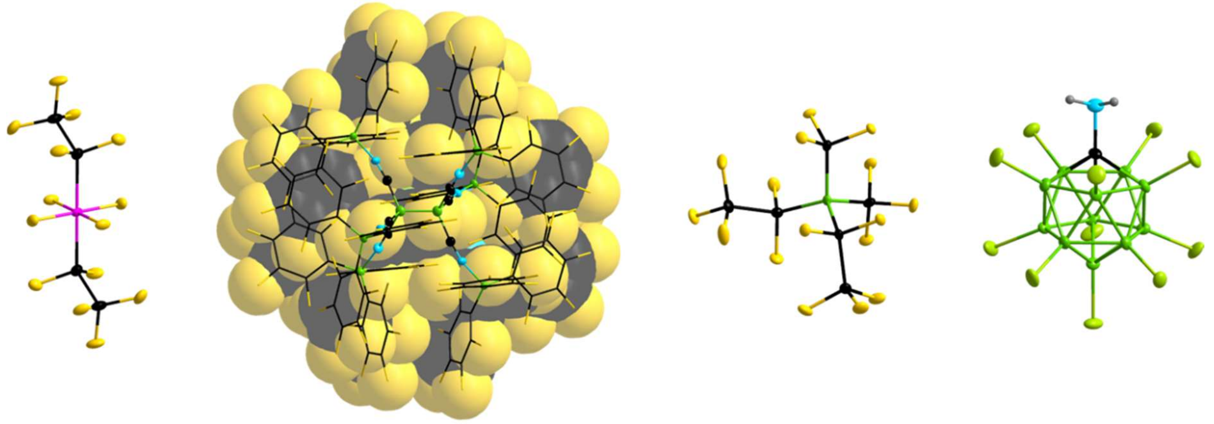

Figure 1: Crystal structures of $[\textit{trans}\text{-}(C_2F_5)_2PF_4]^-$, $[B_2\{CN{\cdot}BCF\}_6]^{2-}$(BCF = $B(C_6F_5)_3$), $[(C_2F_5)_2B(CF_3)_2]^-$, and $[1\text{-}H_2N\text{-}\textit{closo}\text{-}1\text{-}CB_{11}Cl_{11}]^-$.

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Stereochemical Resolution of Polar Subphthalocyanines – A Way to Control Self-Assembly in Liquid Crystals

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Bowl-shaped subphthalocyanines (SubPcs) (Figure 1a,b) are emerging polar semiconductor materials. Among others, they have been employed as new acceptor compounds in organic photovoltaic devices and exhibit an anomalous photovoltaic effect owing to the polar order in their liquid crystal state.[1] The synthesis of the substituted systems **1a-d** results in a 3 : 1 mixture of two enantiomer pairs of regioisomers. Enantiomers and regioisomers impact on the details of their self-assembly.[1-2] Therefore, the efficient separation of all four stereoisomers is of utmost importance.[3-4]

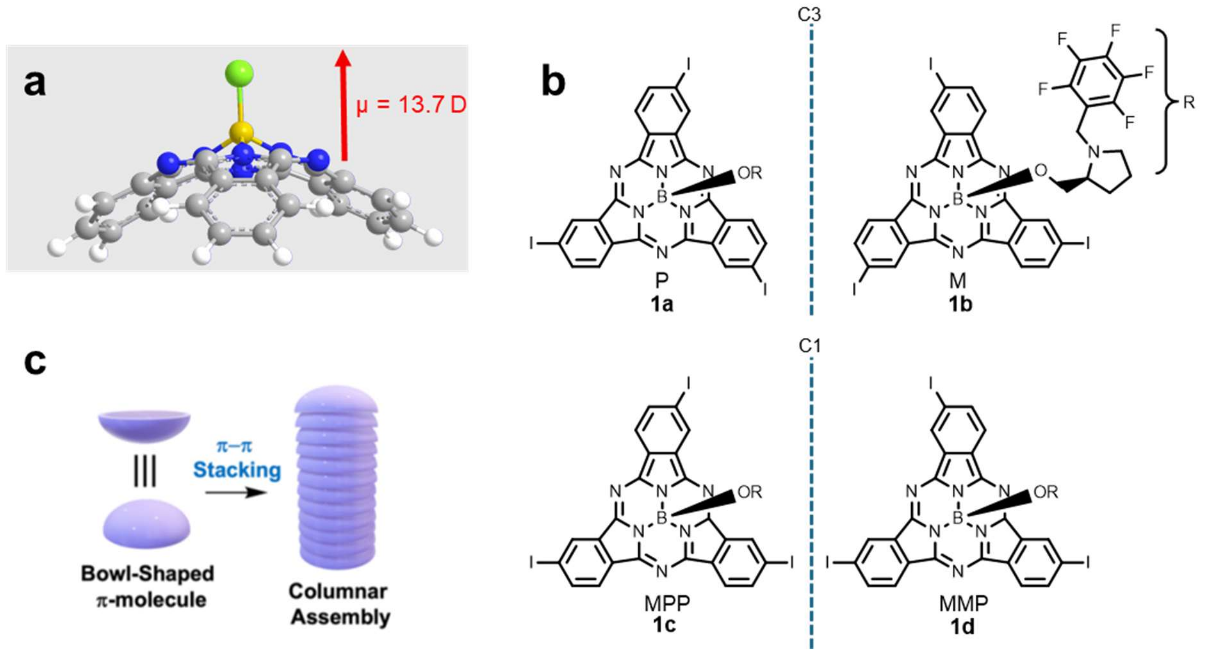

Figure 1: Polar bowl-shaped SubPc (a), C_1- and C_3-symmetric regioisomers and the corresponding enantiomers with a chiral, axial auxiliar (b) and their self-assembly in columnar structures (c).[5]

The present study employs a chiral auxiliary based on the chiral pool (*L*-proline) with an electron deficient pentafluoro-substituted phenyl group which should interact with the aromatic system of the SubPc **1**. The axial substituted diastereomers were obtained in an optimised synthesis and preliminary separation on an analytical chiral HPLC (Chiralpak IC®) indeed revealed the separation of all four isomers. Future work must transfer these results on preparative separation methods.

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Designing new ionizable lipids and targeted PEG-Lipids for the delivery of enhanced mRNA

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Lipidnanoparticles (LNPs) are one of the most common delivery vehicles for the transport of mRNA, and are generally made up of an ionizable lipid, cholesterol, a neutral lipid (e.g. DSPC) and a PEG-lipid. The ionizable lipid is responsible for both the encapsulation of the mRNA and its subsequent release from the endosome into the cell's cytosol where the mRNA payload is translated into proteins. This payload can also be tuned through the untranslated regions (UTR) to increase protein production.

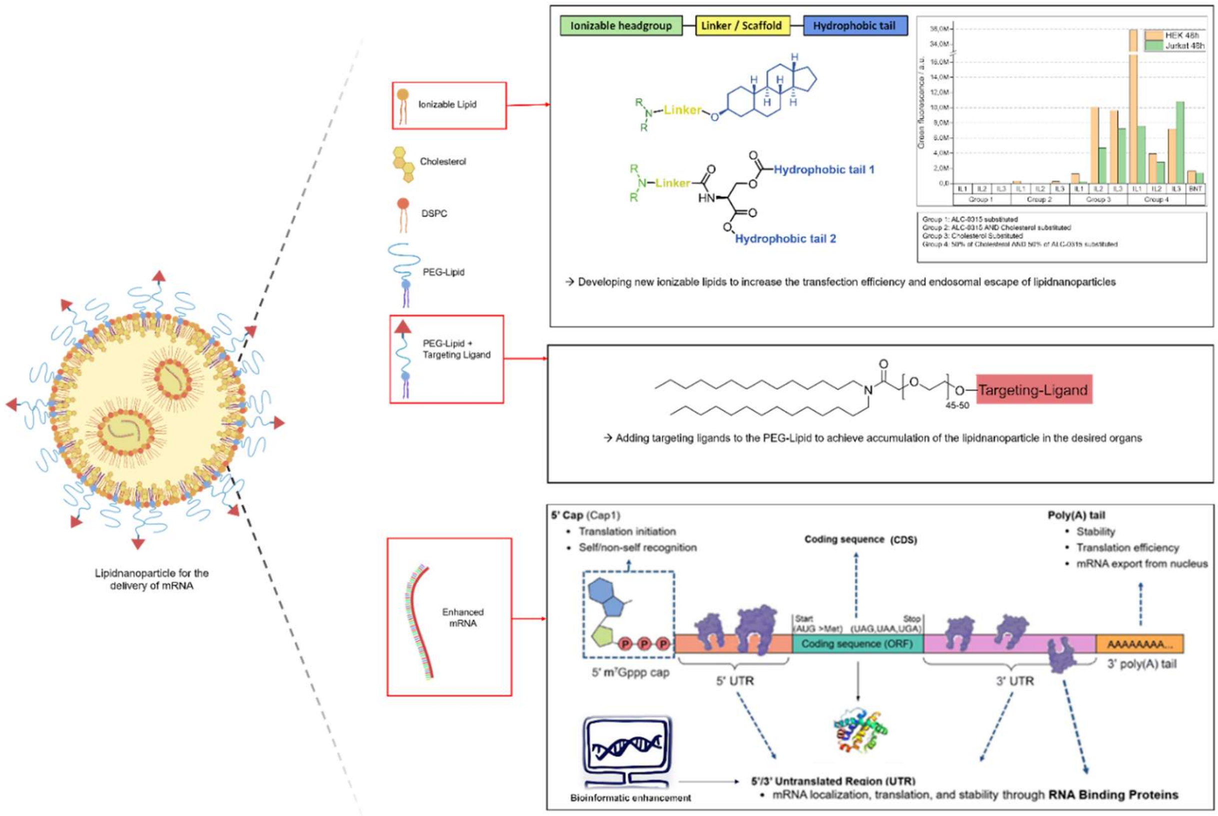

Figure 1: Overview of lipidnanoparticle components, newly developed lipids and mRNA payload.

Despite many significant innovations to make the use of LNPs possible, two main hurdles remain. Firstly, only a small amount of mRNA escapes the endosome, with most of it being either degraded in the endosome or recycled to outside of the cell. Secondly, LNPs are mainly taken up by the liver, which can significantly decrease the efficacy of mRNA therapeutics that target organs other than the liver. To overcome these issues, we are developing new ionizable lipids that aim to increase endosomal escape and transfection efficiency, as well as bioinformatically engineered mRNA sequences to increase translation efficiency. Conjugating targeting ligands to the surface of the LNPs will also achieve higher accumulation in the desired organs.

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Development of an Automated Platform for the Preparation and Characterization of Polyimide Coatings

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Polyimides (PIs) are a class of high-performance polymers that combine lightweight with high chemical resistance and outstanding thermal and electrical insulation. PIs are widely employed as films or coatings for advanced electronics applications. The classic synthesis of PIs relies on toxic catalysts and typically requires organic solvents classified as substances of high concern by environmental regulations.[1] In contrast, our group has developed the synthesis of PIs in water. This approach is composed of an acid-base reaction between a diamine and a tetracarboxylic acid to generate a so-called monomer salt (MS) and its subsequent hydrothermal polymerization.[2,3] The MS systems exhibit ideal 1:1 stoichiometry, are stable, and are prone to form aqueous solutions of high viscosities due to their hygroscopic nature. Aqueous solutions of MSs can be used to form PI coatings and films. However, processing these solutions as coatings prior to PI formation can be challenging and time-consuming due to the many parameters to be considered, e.g., concentration, processing temperature, solution viscosity, etc. These parameters influence features such as coating thickness, and homogeneity and hence affect the quality and performance of the coatings. Furthermore, dozens of MS systems exist, and hence the number of experiments to be performed to generate structure-application parameter-property-relationships is immense. Therefore, methods to automate and optimize the formation and characterization of PI coatings are essential to fully develop the potential of the MSs for PIs processing. Automated platforms have already been applied to optimize films and coatings, yet for fundamentally different materials, e.g., non-fullerene acceptors or perovskite precursor solutions for photovoltaics. Moreover, the platforms used so far do not combine water-based coating processing, in-line characterization, and machine-learning in one fully-automated setup.[4,5]

Herein, we aim at developing an automated platform for PI processing as coatings (**Figure 1**). For the latter a custom-made thermal gradient plate is employed, connected to an automated coating head. This setup allows for efficient screening of different processing parameters. Moreover, the device will be equipped with various in-line characterization techniques, e.g., imaging, and crosscut tests. This will allow for direct assessment of coating properties, enabling data-driven optimization of the process. This approach highlights the power of automation and high-throughput screening in accelerating the development of advanced materials.

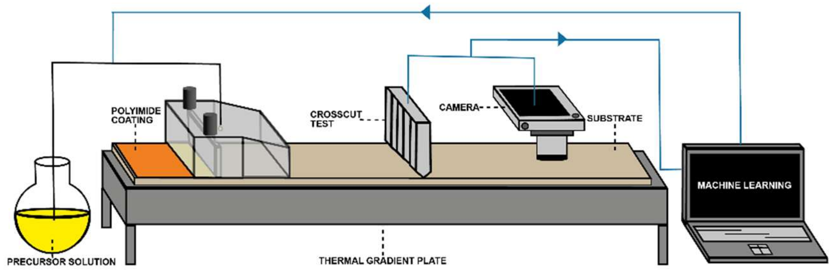

Figure 1: Schematic Overview of the automated coating device.Sezer Hicyilmaz, and A. Celik Bedeloglu, *SN Appl. Sci.* **2021**, *3*, 363.

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.From Text to Test: **Adapting GPT-OSS to Generate Exam-Ready Questions**

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Large Language Models (LLMs) offer new opportunities for supporting learning processes in STEM education, particularly through automated text analysis and content generation. Despite rapid progress in LLMs, their ability to transform raw scientific texts into pedagogically meaningful learning materials remains limited. A central challenge is enabling models to extract the core conceptual content from complex academic sources and convert it into relevant, high-quality questions.

In this project, we investigate multiple strategies for fine-tuning an open-source LLM (GPT-OSS) on consumer-grade hardware to address this challenge.[1] Fine-tuning is performed on curated science-education datasets, combining public resources with a custom chemistry dataset created from OpenStax materials. The model is adapted using Low-Rank Adaptation (LoRA) within a multi-task learning setup to improve both text understanding and question generation.[2]

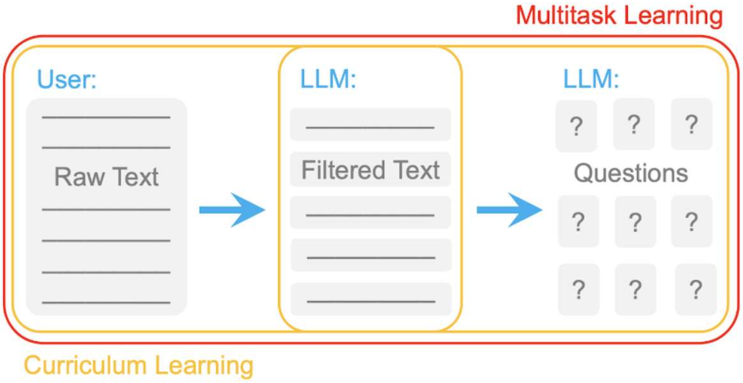

Figure 1: Workflow of the fine-tuned GPT-OSS model: Raw chemistry text is condensed by the LLM into a filtered summary and then used for question generation through a combined multi-task and curriculum-style training approach.

Internal chain-of-thought reasoning improves the structure and conceptual clarity of the generated questions, and our preliminary results demonstrate that domain-specific fine-tuning substantially enhances coherence, relevance, and didactic usefulness compared to the baseline model. These findings highlight the potential of open LLMs for scalable and targeted applications in STEM education.

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Integration of solvation effects for calculating molecules via COSMO/CPCM in Hartree-Fock and SymbolicCI calculations

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The physical state of a molecule strongly influences its chemical behaviour, as reactions, equilibria and spectroscopic properties can differ substantially between a molecule in the gas phase, solid state and solution. Because most chemistry occurs in solution, it is important to account for solvent effects in molecular calculations. Explicit solvent modeling, e.g. treating interactions between a solute and many surrounding solvent molecules using quantum mechanical methods rapidly becomes computationally way too expensive for any but the smallest molecules. Continuum solvation models, such as COSMO [1] or CPCM [2], provide an efficient alternative by treating the solvent as a continuous medium characterized only by its dielectric constant, a measurable property. These approaches replace the explicit solvent molecules with an electrostatic boundary-value problem that yields a linear system of equations for the apparent surface charges. Solving this system is computationally inexpensive and the cost of the solvation step scales approximately linearly with molecular size. As a result, continuum solvation models offer a practical way to incorporate solvent effects into quantum chemical calculations.

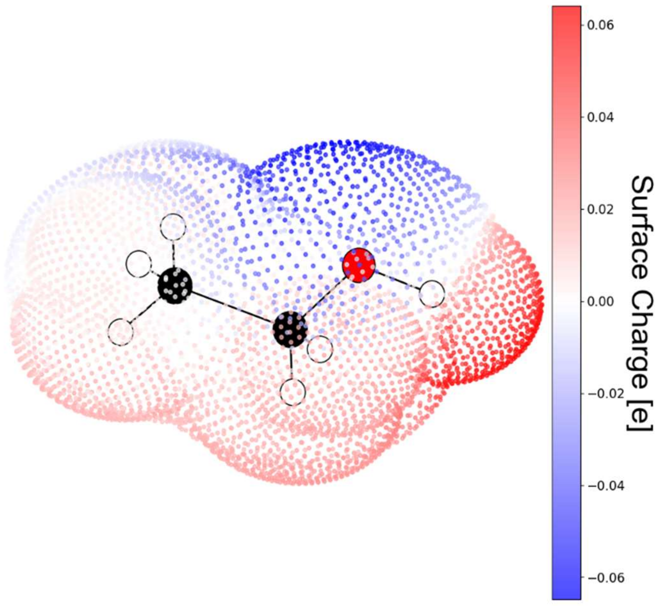

Figure 1: Generated surface cavity with electrostatic potential of Ethanol. Calculated with SymbolicCI using COSMO.

In my bachelor's thesis, I implemented and tested COSMO within SymbolicCI [3], the quantum chemistry program developed in the Röhr group. The goal is to investigate solvent effects on excited states, especially charge-transfer states, which are strongly influenced by solvent polarity. The code is written in the programming language C++ and runs on macOS, Linux and Windows.

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Cyclic diaryl bromanes as molecular carabiner to connect unmodified scaffolds: towards fluorescent peptides

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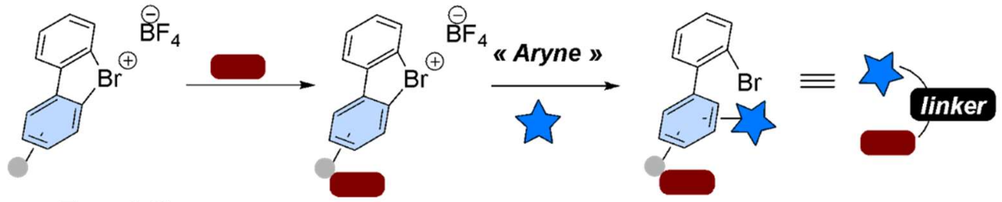
We demonstrate herein a new concept of the use of cyclic diarylbromanes as a unique linker to connect two unmodified scaffolds, as exemplified by the synthesis of fluorescent peptides. This unique reactivity can be achieved in two-step process via initial installation of amino acid esters and peptides on hypervalent bromine via peptidic coupling, followed by metal-free, base-mediated “aryne” type coupling with various fluorophores. Compatibility of this protocol with diversity of amino acid esters and peptides on one hand, and several different amine-containing fluorophores on the other hand, allowed to rapidly access modified peptides under uniquely simple, straightforward and sustainable protocol.



Expectations:

- Use of non-modified substrates
   native functionalities used
- No prefunctionalization steps
- Metal-free
- Mild reaction condition

Figure 1: Illustration of molecular carabiner

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CCyanoborates and Cyanoborate-Modified Polymers

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Cyanoborate anions such as the parent tetracyanoborate anion $[B(CN)_4]^-$ are versatile building blocks for different fields of materials sciences.[1] Because of their high chemical and electrochemical stability in general, and the thermal robustness of their salts with different types of countercations, cyanoborate anions are used as components for electrolytes, e.g. for supercapacitors, metal-ion batteries, and dye-sensitized solar cells (DSSCs).[1] Salts with cyanoborate anions include metal salts, transition metal complexes, and salts with organic cations. With large unsymmetrical organic cations cyanoborate room temperature ionic liquids have been developed that provide very low viscosity, high conductivity, and low melting points in combination with high chemical, electrochemical, and thermal stability.[1–3] Cyanoborate anions also serve as starting compounds for further (cyano)boron compounds.[1] This includes the weakly coordinating $[B(CF_3)_4]^-$ anion,[4,5] boron-centered dianionic nucleophiles (e.g. $B(CN)_3^{2-}$, $BR(CN)_2^{2-}$),[6] and tricyanoborane-functionalized anionic *N*-heterocyclic carbenes (anionic NHCs).[7,8] Especially, $B(CN)_3^{2-}$ and related boron-centered dianionic nucleophiles are promising starting compounds for the introduction of anionic boron moieties. Many otherwise hardly accessible cyanoborate anions, e.g. $[B(CN)_3(CO_2H)]^-$,[6] $[(C_6H_{5-n}F_nB(CN)_3]^-$,[9] the diborane(6) dianion $[B_2(CN)_6]^{2-}$,[10,11] and $[Pb\{B(CN)_3\}_4]^{4-}$,[12] were obtained via nucleophilic substitutions. The anionic $B(CN)_3$ moiety was introduced into polymers leading to ionomers that are potential solid electrolytes for electrochemical devices, e.g. metal-ion batteries. A further example are beads decorated with tricyanoboryl substituents for ion exchange chromatography. Two different synthetic strategies were applied, (i) the reaction of a prefunctionalized polymer or bead with $B(CN)_3^{2-}$ or (ii) polymerization of a $B(CN)_3$-functionalized styrene monomer.

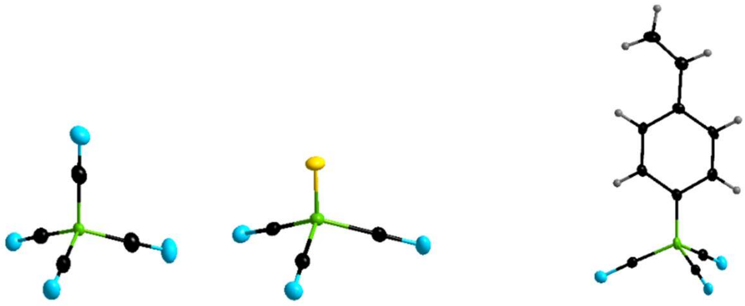

Figure 1: Crystallographic structures of $[B(CN)_4]^-$, $[BF(CN)_3]^-$ and $B(CN)_3$-functionalized styrene.

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Silylated Model Compounds for Covalent Incorporation into Silica Fibers for Drug Delivery Applications

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Glioblastoma is an aggressive and malignant brain tumor with notably high mortality rates[1] and limited alternatives of treatment that only extend the patients' lifespan for a short period. One main obstacle in glioblastoma treatment is the blood-brain barrier (BBB), which prevents drugs from reaching the brain.[2] As a result, drug delivery across the BBB has become a central focus of research to improve chemotherapeutic outcomes. One approach is local drug delivery systems, which do not rely on systemic administration via bloodstream or oral ingestion,[3] and hence can be considered for direct application to the tumor margin. In this context, nanoparticle-containing hydrogel materials that encapsulate therapeutic agents within porous structures have been investigated. The effectiveness of such hydrogels for drug delivery nonetheless remains limited due to negligible effects on survival rates and uncontrolled drug release.[3,4]

Silica-based carriers with covalently attached therapeutic agents have been explored as promising platforms for drug delivery.[5] These materials are derived from organosilanes of the type $Si(OR^1)_x(R^2)_y$ (which have negative impact on human health) and hence Si-C bonds alongside Si-O bonds arise in the final SiO_2-based materials. The drug component is typically connected via the Si-C motifs. Alternatively, silica fibers featuring exclusively silicon-oxygen (Si-O) bonds have been investigated as scaffolds for health applications such as wound dressings.[6] These systems, made from alkoxysilanes, are biocompatible and benign to human health. Furthermore, while Si-C bonds are not biodegradable under physiological conditions, i.e. they do not cleave in the human body, the use of Si-O bonds results in a material that undergoes degradation through hydrolytic cleavage under physiological conditions and produces biocompatible products, i.e., orthosilicic acid.[6]

In this work, we aim to compare the release of small molecules that are physically encapsulated within a silica matrix to those covalently linked (Figure 1). Covalent attachment is expected to result in release kinetics that are controlled by the hydrolysis of Si-O bonds during degradation of the fibers. To test this without using expensive and toxic cytostatic agents, we synthesized a silylated coumarin dye as a model compound to analyze the release profiles. In this contribution we discuss the synthesis and characterization of these materials, setting the basis for subsequent work on integrating active pharmaceutical molecules via similar chemistries.

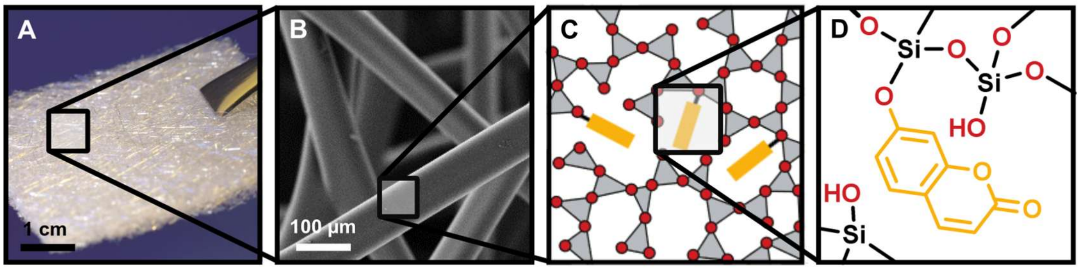

Figure 1: **A.** Biodegradable silica fiber pad, **B.** scanning electron microscopy image showing the fibrous morphology, **C.** schematic representation of the dye covalently attached to silica network, **D.** chemical structure of coumarin dye covalently bound to silica.

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Excitonic Reststrahlen Effect in Ruddlesden–Popper Perovskites

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Layered Ruddlesden–Popper perovskites (RPPs) ($(RNH_3)_2(A)_{n-1}M_nX_{3n+1}$) are an exciting class of materials made of alternating organic and inorganic layers. This natural quantum well structure, allows for strongly confined excitons, bound pairs of electrons and holes, with very high oscillator strengths.[1] These properties makes them ideal model systems for studying strong light-matter interactions and the formation of so-called exciton-polaritons in these materials.[2] In this work, an excitonic Reststrahlen effect, a phenomenon in which strong exciton resonances induce a reflectivity band near unity, was identified and characterized in phenethylammonium lead iodide (PEPI). Transfer-Matrix-Method (TMM) simulations of the thin film were employed to fit temperature-dependent transmission measurements to a Lorentz oscillator model and to extract the dielectric function of the material.

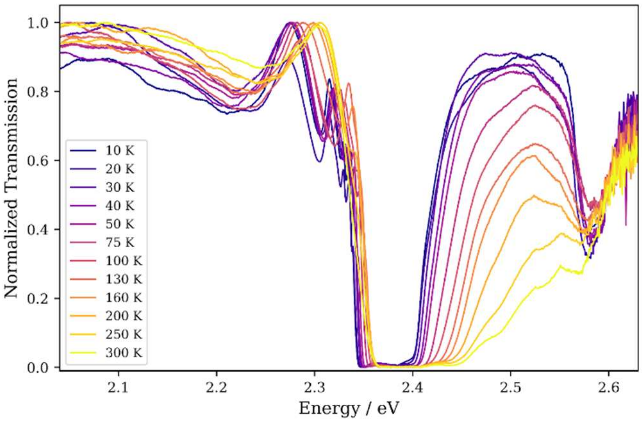

Figure 1: Normalized transmission spectra of PEPI at various temperatures.

This dielectric function showed a clear region where the material’s permittivity becomes negative, a defining property of the Reststrahlen effect and suggested an unusual optical behaviour called hyperbolic dispersion. By further modelling the electric field and resonance modes in the film, we observed polariton-like excitations with strong longitudinal field components. These findings not only deepen our understanding of light–matter coupling in layered perovskites but also point toward possible applications in advanced nanophotonic devices and metamaterials.[3][4]

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Macrocycles as innovative scaffolds in modern drug discovery

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Macrocyclic compounds have emerged as a promising class of drug candidates capable of bridging the gap between small molecules and biological therapeutics. While traditional drug discovery has largely been guided by Lipinski's Rule of Five, recent advances highlight that macrocycles can maintain cell permeability and even oral bioavailability despite exceeding Ro5 limits. This unusual property is often attributed to their molecular chameleonicity, the ability to adapt their conformation and polarity depending on the surrounding environment. Such behavior enables macrocycles to balance solubility in aqueous media with membrane permeability and to address "undruggable" targets that are inaccessible to conventional small molecules. [1,2,3]

In this project, distinct building blocks were used to generate a library of macrocycles with optimized physicochemical properties for improved cell permeability. Each building block was selected based on key design principles such as lipophilicity, limited hydrogen bond donors, ring size, rigidity, and the inclusion of structural motifs like phenyl rings and tertiary amines to promote passive diffusion across membranes.

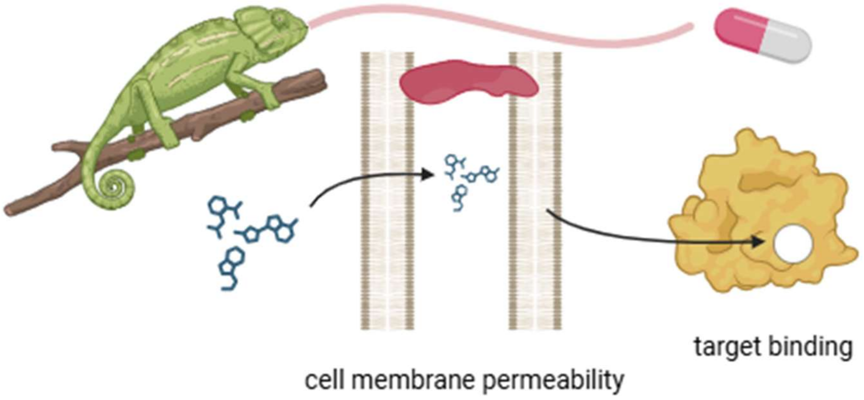

Figure 1: Chameleonicity in drug design: balancing cell permeability and target binding.

The macrocycles are synthesized via solid-phase peptide synthesis, followed by lactamization to achieve efficient macrocyclization. This modular approach enables systematic variation of ring size, polarity, and conformational rigidity, allowing fine-tuned control over ADME-related properties such as cell permeability and metabolic stability.
By applying this strategy, the study aims to expand the accessible chemical space for drug discovery beyond the traditional Rule of Five, facilitating the development of novel scaffolds capable of targeting challenging intracellular proteins.

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Towards a Fully Automated Closed-Loop Hydrothermal Flow System

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The use of green reaction media in organic synthesis contributes to more environmentally friendly chemical practices. Among these, water stands out as a non-toxic, abundant solvent whose physicochemical properties can be tuned by varying temperature and pressure. Consequently, hydrothermal synthesis has emerged as a valuable and greener alternative to conventional methods for numerous organic transformations.[1]

Optimizing reaction parameters is essential for developing efficient and sustainable syntheses, yet traditional manual experimentation remains time-consuming and resource intensive. Flow chemistry addresses these limitations by enabling precise control of reaction conditions, continuous operation, and real-time analysis. When combined with computational algorithms, it allows for data-efficient, scalable, and systematic exploration of the reaction space, which represents a key step towards self-driving laboratories that accelerate discovery while minimizing human intervention.[2]

In this work, the principles of autonomous flow chemistry are applied to hydrothermal synthesis through the development of an automated high-pressure, high-temperature flow platform. This approach illustrates how integrating flow chemistry, automation, and machine learning can accelerate the development of sustainable chemical processes. Using algorithms, such as Bayesian optimization, and in-line spectroscopic techniques for continuous monitoring enables rapid identification of optimal conditions. Within this framework, an optimization workflow was established to advance towards self-driving experimental systems capable of autonomously optimizing reactions and improving efficiency and sustainability in chemical research. Current efforts aim to realize a fully self-optimizing robotic flow platform capable of autonomously executing and refining chemical syntheses with minimal human intervention, as illustrated in Figure 1.

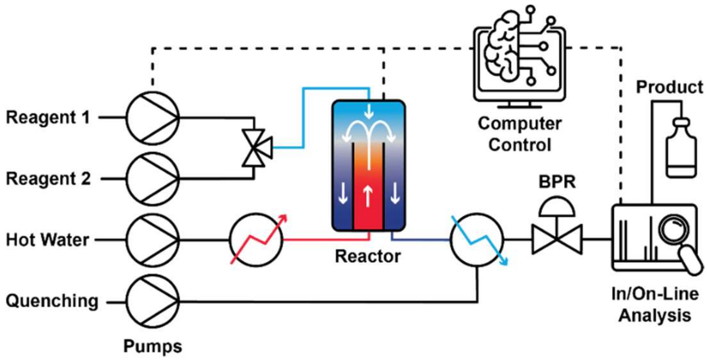

Figure 1: Schematic overview of the autonomous experiment workflow in the high-pressure flow platform.

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Reductive Decationizable Polycarbonates for Targeted mRNA Delivery

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The delivery of mRNA represents a potent and adaptable approach for the development of the next generation of therapeutic treatments. Current lipid-based delivery systems, while proven effective, are limited in their implementation owing to a range of physicochemical properties preventing long-term storage and reconstitution, intrinsic immunostimulatory properties in addition to difficulties in precise targeting and controlled release of mRNA payloads. For the aforementioned reasons, cationically charged polymers are being considered as alternative carriers to lipid formulations [1].

Herein we develop a biodegradable aliphatic polycarbonate parent polymer bearing pendant alkyl thiosulfonates able to undergo rapid disulfide formation with thiol bearing aliphatic amines able to ionically complex mRNA. Parent polymers with narrow molecular weight dispersities were generated via controlled ring opening polymerization of an alkyl thiosulfonate cyclic carbonate monomer, endgroup modification with PFP carbonate allowed for relevant fluorescent dye labelling [2].

The thiosulfinate pendant groups could then be quantitatively converted into the corresponding disulfide upon introduction of suitable thiol containing amine salts while minimising unwanted interchain coupling. Successful mRNA complexation of the generated amine polymers was then evidenced by gel electrophoresis at low N/P ratios. Polymer formulations were then used to successfully monitor cell uptake and transfection with mRNA encoding the Green fluorescent protein (GFP) while displaying limited cell toxicity.

Specific cellular targeting was realised by the formation of a block co polymer consisting of the already established polycarbonate/amine block and a PEG block bearing a clickable azide functionality. Subsequently, attachment of a DBCO modified targeting moieties can be achieved via strain promoted azide alkyne click (SPAAC) chemistry with an envisioned application in specific cellular targeting for the treatment of atherothrombosis [3].

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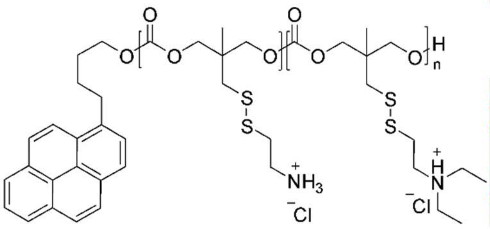

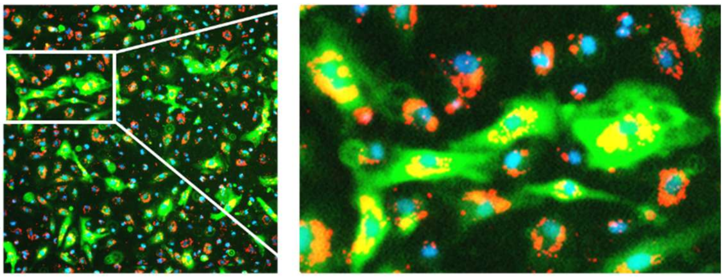

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IMIDAZOLYL-FUNCTIONALIZED BORON CLUSTERS: BUILDING BLOCKS FOR ANIONIC *N*-HETEROCYCLIC CARBENES AND MORE

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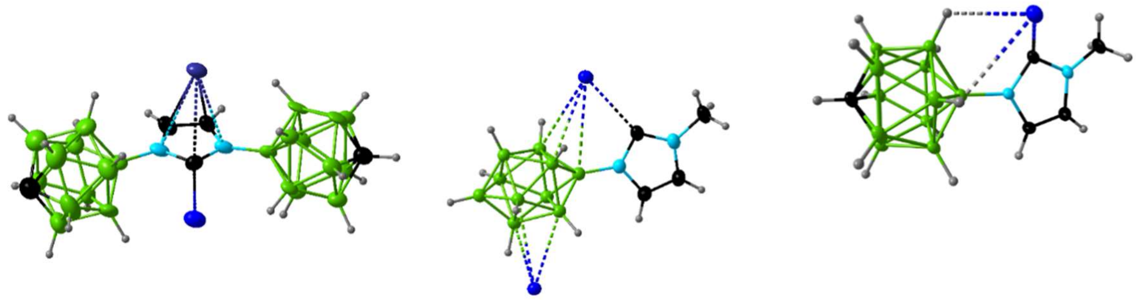
Since their first isolation by Arduengo in 1991, *N*-heterocyclic carbenes (NHCs) have emerged as an important class of compounds in various fields of chemistry.[1] Owing to their unique electronic characteristics - strong σ-donor and π-acceptor properties - they enable a wide range of applications, for instance, in organocatalysis and transition-metal catalysis.[1b] The chemical structure of an NHC provides several positions for functionalization, particularly at the nitrogen atoms.[1b] Following the synthesis of 1,3-diadamantylimidazol-2-ylidene by Arduengo, numerous NHC derivatives have been developed over the past three decades.[1b] A smaller subgroup within this class comprises anionic NHCs.[2] Among these, the most notable are those featuring anionic, non-delocalized substituents derived from group 13 elements, particularly boron.[2] In recent years, we have contributed to this field through the synthesis of the anionic NHC 1-methyl-3-(tricyanoboran)imidazol-2-ylidene and the dianionic NHC 1,3-di(tricyanoboran)imidazol-2-ylidene.[3] We demonstrated that functionalization of NHCs with the strong Lewis base tricyanoborane leads to enhanced stability and significantly increases both σ-donor and π-acceptor capacities compared to related unsaturated NHCs reported in the literature.[3] Building on these studies, we have pursued the synthesis of boron cluster-functionalized NHCs. Due to their exceptional stability, steric bulk, and delocalized electron density, boron clusters represent ideal substituents for NHCs and offer versatile opportunities for further functionalization.[4] Over the past years, we have successfully synthesized a series of *closo*-decaborate- and 1-carba-*closo*-dodecaborate-functionalized imidazoles, which were subsequently deprotonated to yield the corresponding NHCs using suitable bases. Furthermore, we isolated a di-(1-carba-*closo*-dodecaborate)-substituted NHC as well as several 1,10-di(imidazolylidene)-*closo*-decaborates. Our further investigations revealed that the incorporation of boron clusters significantly enhances the σ-donor capacity of these NHCs, opening new perspectives for different applications.



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Designing Macromolecular Therapeutics for Immunoengineering

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At the interfaces between chemistry, materials and life sciences, we are investigating novel polymeric drug carriers that specifically target body's own self-healing mechanisms. In this regard, nano-sized carriers have proven to be particularly advantageous, especially for preventive vaccinations or immunotherapeutic cancer treatments: They provide several characteristic features such as size and multivalent surface properties to which the immune system is particularly sensitive.

For that purpose, we synthesize functional monomers, polymerize them into multifunctional block copolymers, and finally formulate them into biodegradable polymeric nanoparticles. Such carriers are able to release their immunostimulatory cargo through biological stimuli (pH, reduction equivalents, enzymes) only at their site-of-action, thereby increasing drug efficacy while circumventing systemic side effects.

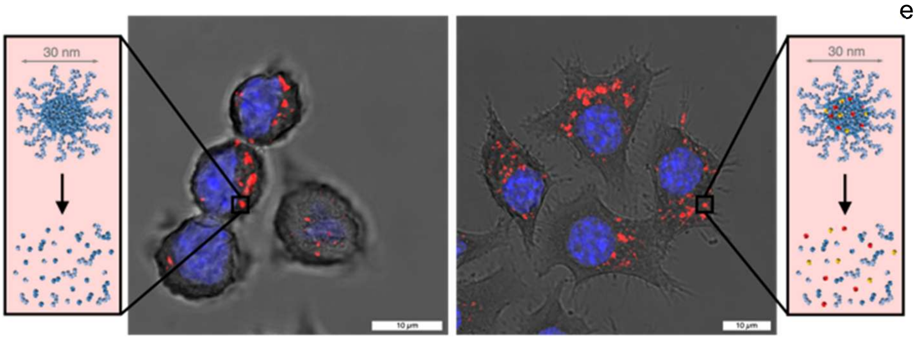

Figure 1: Polymeric nanoparticles (red) can be taken up by immune cells (cell nucleus blue) and then get degraded (left). If they contain an immune modulatory, this drug can sneak into the immune cells and wake them up from their sleepy (immune suppressive) state (right).

Our team has recently moved into the Center of Polymers of Life at the JMU Würzburg and is offering opportunities for ambitious bachelor or master thesis projects as well as PhD positions. Beyond advanced organic and macromolecular syntheses, we pay careful attention at biophysicochemical characterization methods as well cell biological in vitro assays. They are required prior to further in vivo immunobiological studies together with our cooperation partners from medicine and immunology. Altogether, in an interdisciplinary research team we aim at understanding and improving drug performance by our nanocarriers and, thus, path their way towards advanced immunotherapeutic nanomedicines.

Further infos:
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.Photodissociation Dynamics of the Bromomethyl Radical

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Bromomethyl belongs to the class of organic halogen radicals. Therefore, it can potentially influence the atmosphere by reacting with the ozone layer and causing its depletion similar to HCFCs. The photoionization of bromomethyl was already investigated by several groups, including Steinbauer and coworkers.[1] They determined the ionization energy and structure with VUV synchrotron radiation and investigated the dissociative photoionization. To obtain further insights into the dissociation of bromomethyl, we analyzed the fragments of the radical using velocity map imaging (VMI).

CH2Br-NO2 was used as a precursor for the halogenated methyl radical, because the weaker C-NO2 bond can be cleaved through pyrolysis. Subsequently, laser light with 235 nm was deployed to dissociate the formed CH2Br radical. The major dissociation pathway gave the methylene and bromine fragments which were detected with SPI at 118 nm and [1+1']-REMPI at 356 nm respectively. With velocity map ion imaging, the translational kinetic energy distribution of the photofragments was determined. The recorded images of the bromine and methylene photofragments showed an anisotropic distribution, implying a direct dissociation.

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Hyperspectral Photoluminescence Imaging of Two-Dimensional Perovskites

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Two-dimensional hybrid perovskites such as phenethylammonium lead iodide $(PEA)_2PbI_4$ (short PEPI) have attracted growing interest for their exceptional optical properties and tunable electronic structure. Their layered nature gives rise to excitonic resonances and possibly spatially varying emission characteristics, especially in exfoliated flakes, at their edges or in stacked heterostructures. Local variations in thickness, strain, or composition can strongly affect the photoluminescence (PL) response, yet conventional spectroscopy averages over these features. To resolve such inhomogeneities, spatially and spectrally resolved methods are required. A hyperspectral PL imaging setup was developed to record emission spectra with both high spatial, spectral and - if desired - picosecond temporal resolution. First measurements on exfoliated PEPI flakes of varying thickness demonstrate that the setup can detect position-dependent spectral shifts and intensity variations.

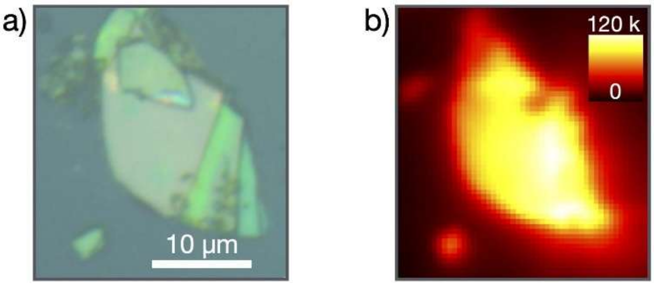

Figure 1: Images of the same exfoliated perovskite crystallite. (a) Optical microscope image recorded at 50× magnification. (b) Photoluminescence (PL) map showing the spectrally integrated emission intensity in the range 500–560 nm.

The system provides a foundation for future studies of spatially varying optical phenomena such as edge states, interlayer coupling, and heterostructure interfaces[1-3]. Although currently limited to room-temperature operation, this platform opens the door to systematic investigations of local band-gap variations and excitonic processes in two-dimensional perovskites. In the long term, such insights may guide the design of more uniform and efficient optoelectronic devices based on layered perovskite architectures. The data acquisition and image evaluation were performed using a custom Python-based software developed in-house, which is available on GitHub[4].

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Functionalized Polyimides for Electrochemical Applications

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Polyimides (PIs) are a class of high-performance polymers, since their discovery PIs have mainly found application for their high thermal stability and inertness, e.g. as insulants in spaceships. However, their vast chemical design space and therefrom arising variety in physicochemical properties makes them promising candidates for a number of other applications. In particular PIs have shown great potential in batteries, where their incredible versatility is highlighted by the fact that PIs can be used for almost any part, including electrodes, electrode coatings, separators or membranes, binders, electrolytes and even current collectors.[1,2] In the case of cathodes, PIs provide good cycling stability but are limited in their redox potential and thereby power delivery, especially compared to established inorganic materials. To overcome this liability is the goal of this project.

Tuning of the Redox Potential by Adjusting the Aromatic Moiety

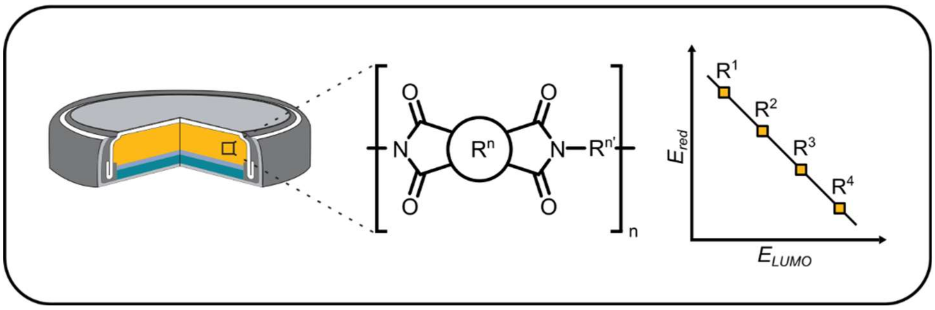

Figure 1: Graphical illustration of the project's goals. Adjusting the aromatic core and connected functionalities allows for targeted tuning of the HOMO and LUMO energies. For cathodes specifically a lower LUMO will result in a higher reduction potential.

For cathode materials the redox potential is governed by the LUMO level. Therefore, increasing the aromatic delocalization will in turn lead to a higher redox potential.[3] A larger aromatic core, however, will decrease the specific capacity and also complicate processability due to a decrease in solubility. Alternatively, the LUMO level may be adjusted by introducing functional groups to the carbon backbone. This approach has been successfully demonstrated for bisimides but and shown to work in principle for the corresponding polymers.[4,5] However, a conclusive study on the influence of different functional groups on the electrochemical performance of the final PIs has so far not been reported. Performance of organic electrodes is not only decided by the redox potential. Ionic functionalities have been found to effectively increase the ionic transport number without the addition of filler material, increasing the effective capacity and decreasing energy losses.[6] The goal is therefore not merely to evaluate the potential of the materials but also the overall performance of the resulting batteries.

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