

Vorstellung der Preisträger und Preisträgerinnen des Römer-Preises 2021

Mit herzlichem Dank an die Römer-Stiftung
für die großzügige Förderung
der Departments Biochemie und Chemie.



Mit Preisen in Höhe von 1.000 €
wurden für exzellente Leistungen
während ihrer Master-Arbeiten

ausgezeichnet:

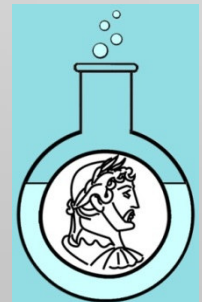
Florian Burkert

Marian Ebeling

Yannick Lemke

Patrick Schüler

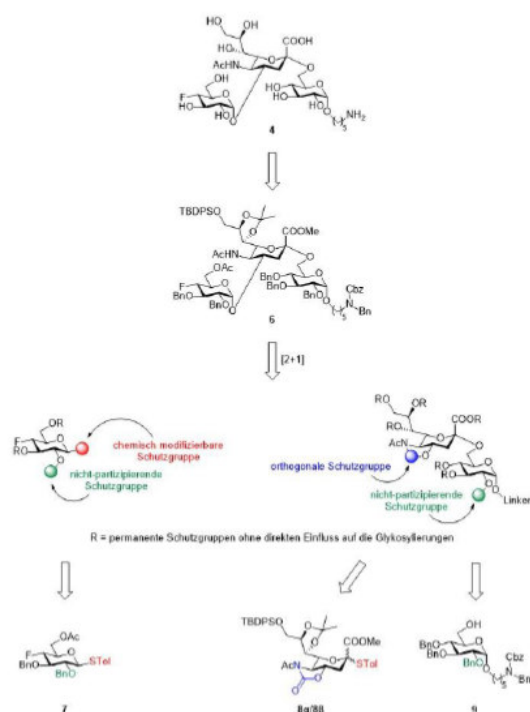
Mirjam Zipkat



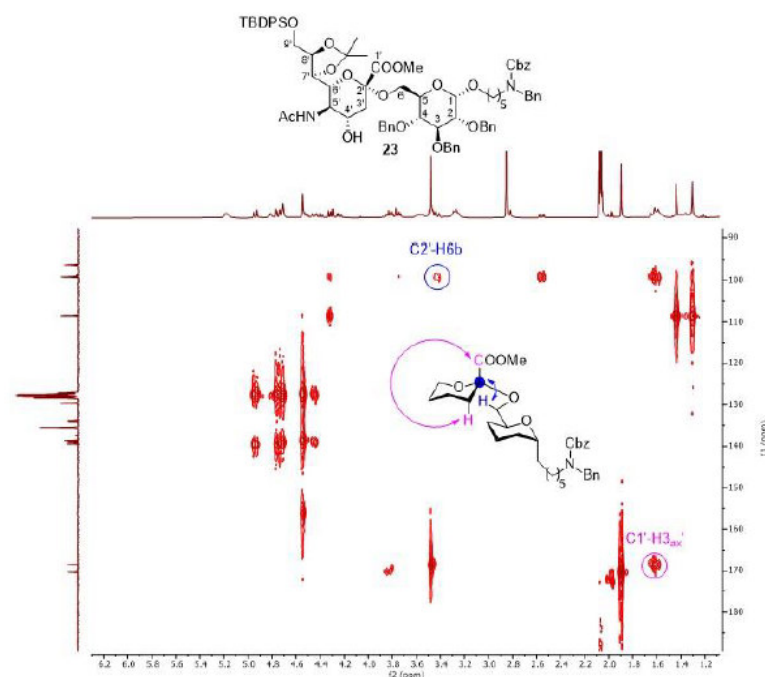
Synthesestudien zum Aufbau chemisch modifizierter Analoga der kapsulären Polysaccharidstruktur von *Neisseria meningitidis* Serogruppe Y

Masterarbeit von Florian Burkert

Unter der Leitung von Sebastian Neidig im Arbeitskreis von Prof. Dr. A. Hoffmann-Röder



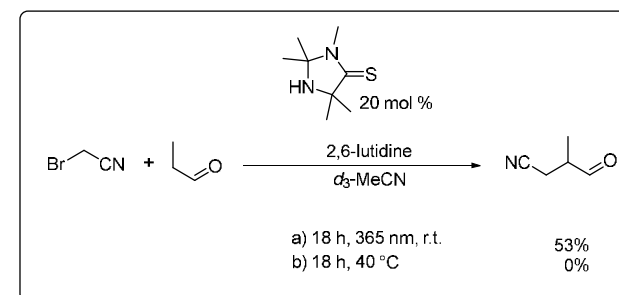
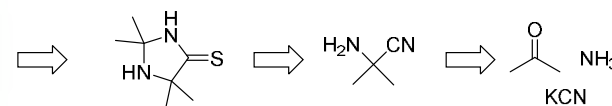
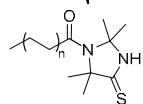
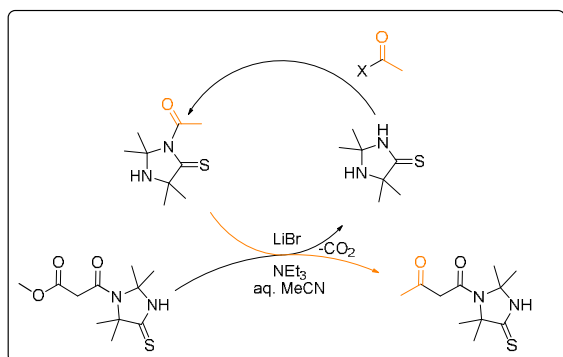
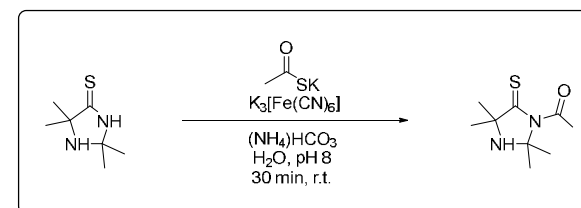
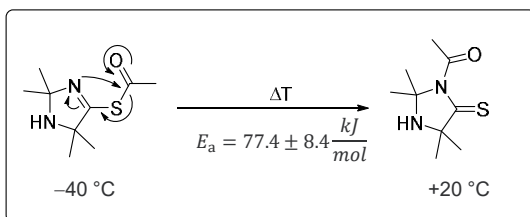
Darstellung der Schutzgruppenanforderungen und Schlüsselbausteine zur Synthese des fluorinierten Trisaccharids **4**.



Ausschnitt aus dem HMBC-NMR-Spektrum des Disaccharids **23**.

Prebiotic Emergence of Fatty Acids and Catalytic Activity Induced by the S- and N-Functionalized Imidazolidine-4-thione Scaffold

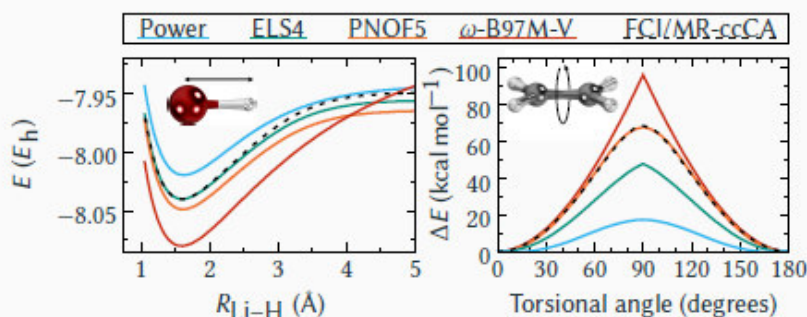
Marian Ebeling
AK Trapp



Time-Dependent, Integral-Direct Reduced Density Matrix Functional Theory for Massively Parallel Architectures

Yannick Lemke
AK Prof. Ochsenfeld

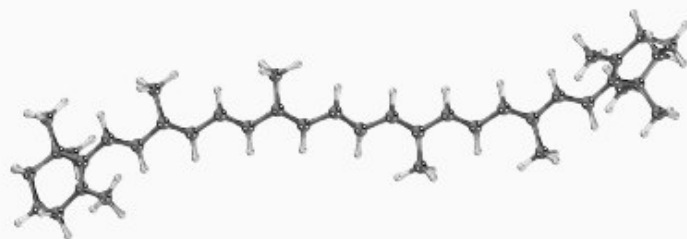
Static correlation



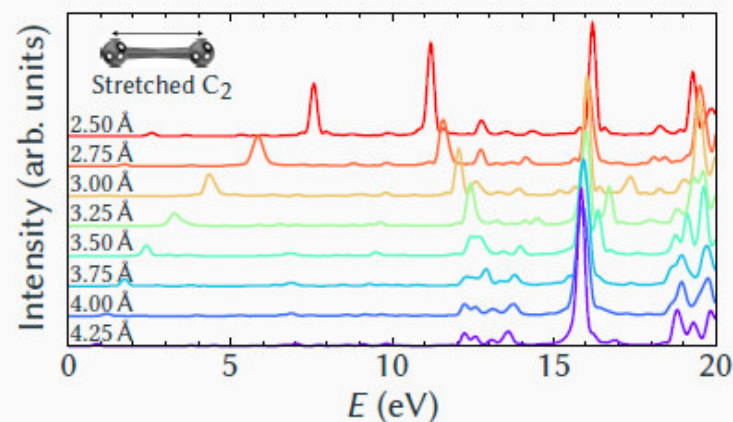
RDMFT

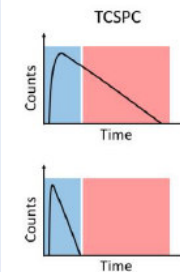
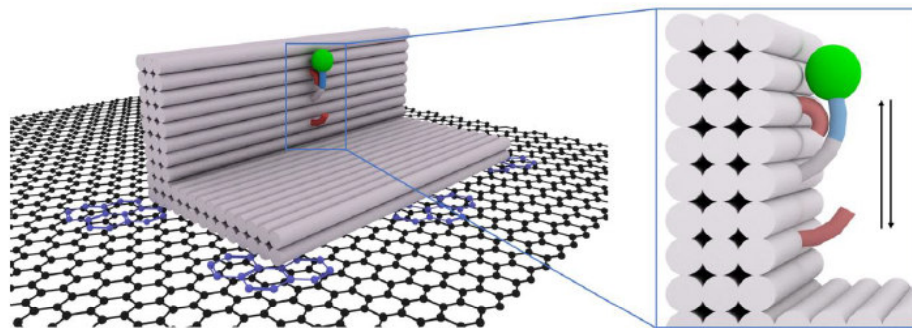
Integral-direct RDMFT

- Development of new AO-based algorithms
 - Efficient implementation @ CPU/GPU
- Large systems & basis sets
(e.g. β -carotene @ def2-TZVP)

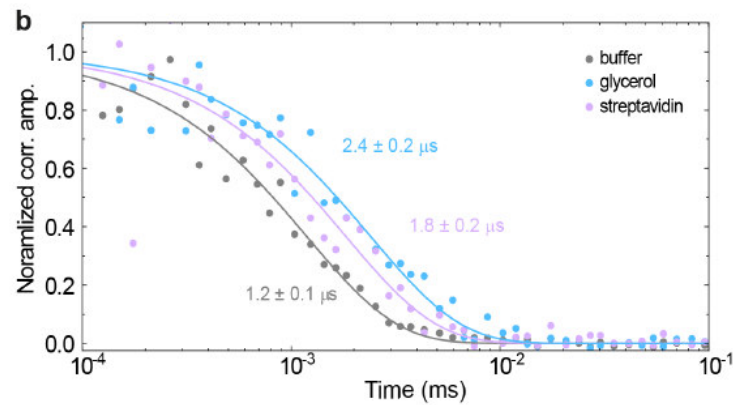
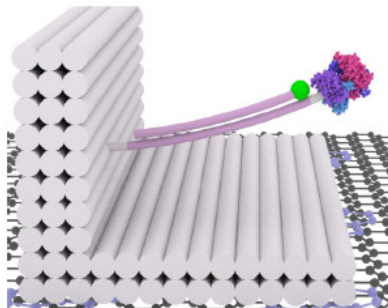


Time-dependent RDMFT: UV spectra



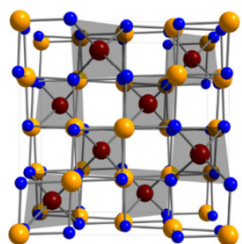


a tether + recognition

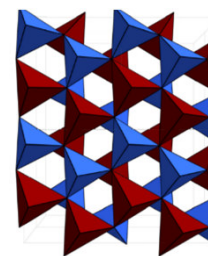


Patrick Schöler
AK Tinnefeld

Synthesis of Tin Nitride Semiconductor Materials



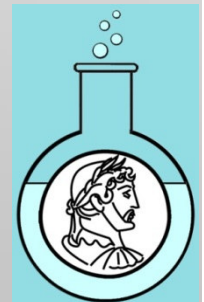
Mirjam Zipkat
Schnick group
Solid-State and Materials Chemistry



Promotions-Preise in Höhe von 2.500 €
wurden für herausragende Leistungen verliehen an:

Stefan Bauernfried
Dr. Anna Closs
Dr. Johannes Dietschreit
Van Hoan Do
Dr. Daniel Graf
Wilhelm Greulich

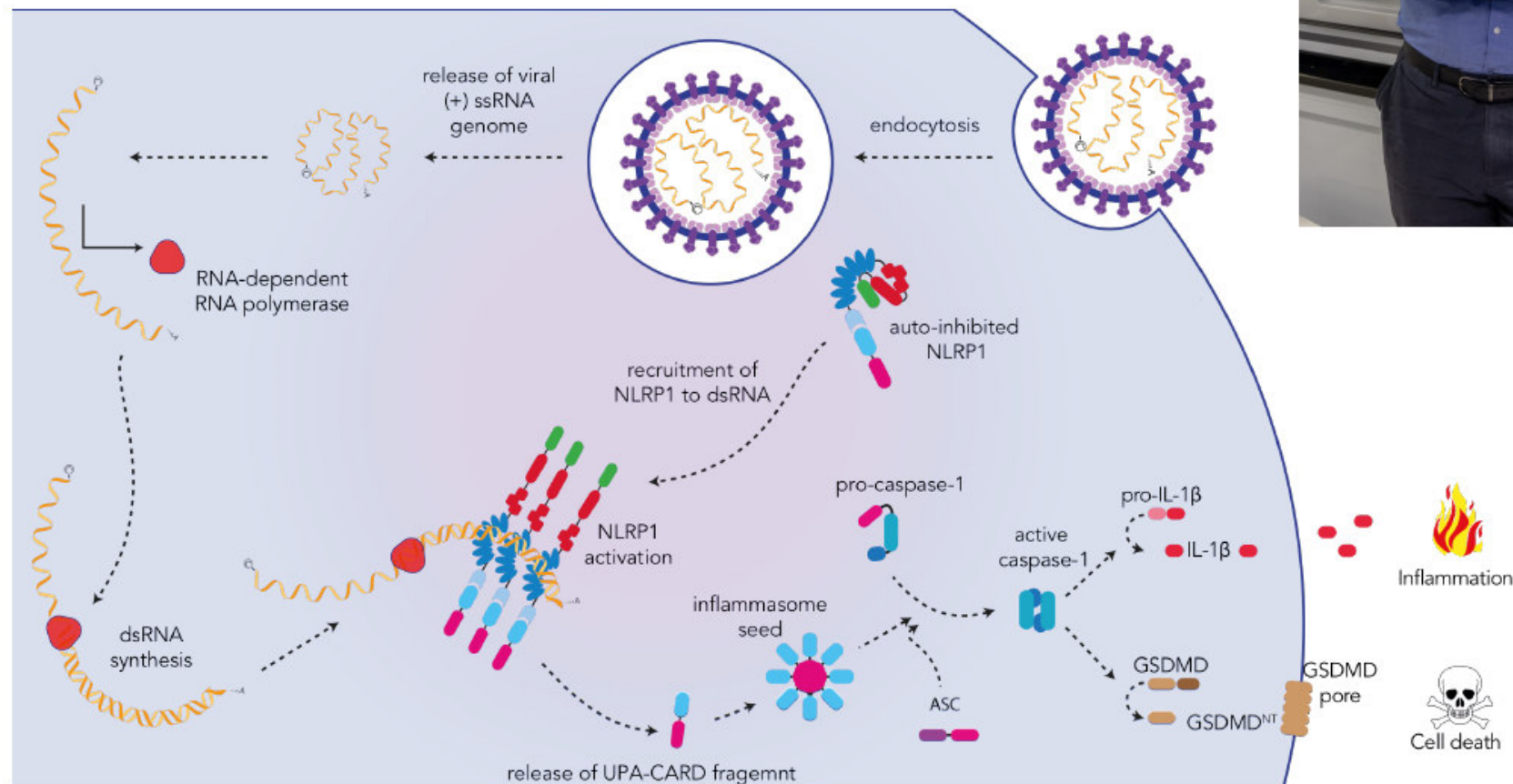
Johannes Harenberg
Hannah Reinking
Dr. Thomas Schnappinger
Kristina Stakyte
Dr. Valentin Weippert



Stefan Bauernfried - AG Hornung

Innate Immunity

Human NLRP1 is a sensor for double-stranded RNA

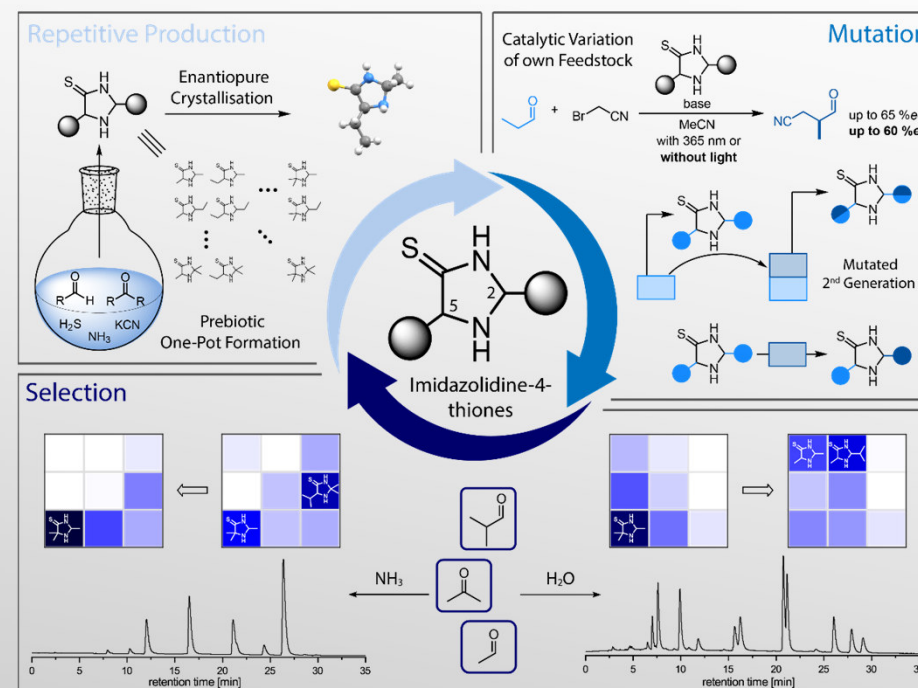
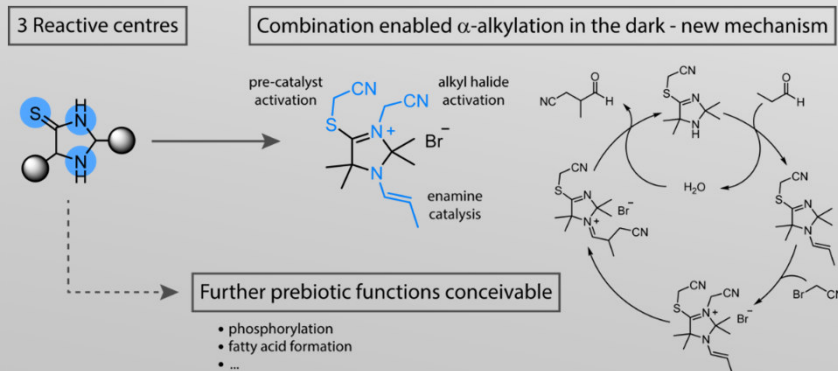




Dr. Anna Closs
AK Prof. Dr. Oliver Trapp

Forschungsarbeit in der organischen Chemie:

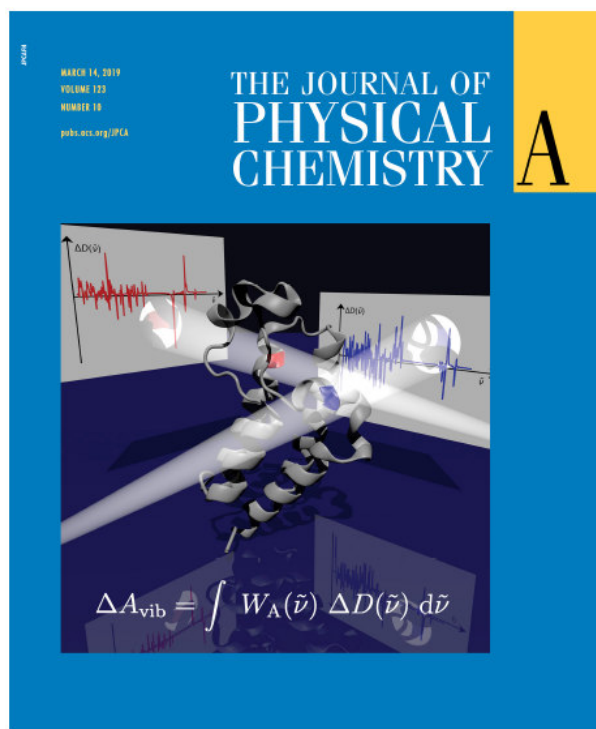
Identifizierung von Imidazolidine-4-thionen als vielversprechende präbiotische Organokatalysatoren.
Realisierung und mechanistische Untersuchung der organokatalysierten α -Alkylierung von Aldehyden sowie einer ersten Form der molekularen Evolution auf der frühen Erde.



A. C. Closs, E. Fuks, M. Bechtel, O. Trapp, *Chem. Eur. J.* 2020, 26, 10702-10706.

A. C. Closs, M. Bechtel, O. Trapp, *Angew. Chem.* accepted.

Dr. Johannes Dietschreit



AK Ochsenfeld

Theoretische Chemie

Advanced Techniques for the
Computer Simulation and
Analysis of Biomolecular
Systems



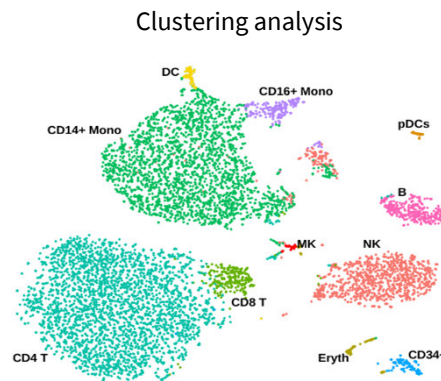
Computational methods for large scale scRNA-seq and multimodal omics data



Van Hoan Do
AK Canzar, Gene Center

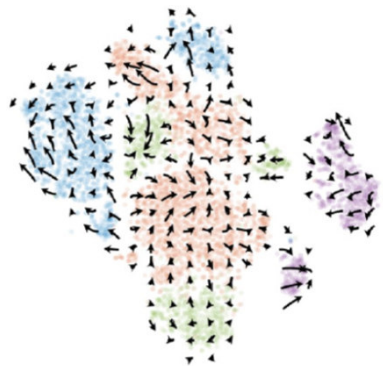
Research Area:

- Computational biology
- Single cell data analysis
- Big data analysis
- Machine learning, optimization



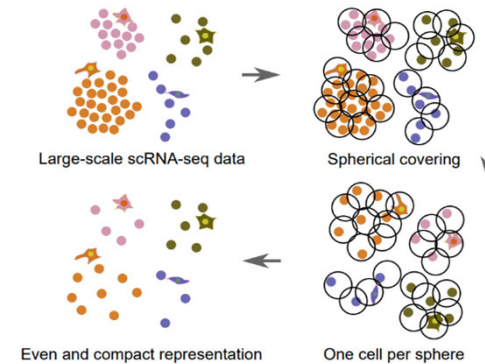
Do et al., Genome Research 2021

Data visualization



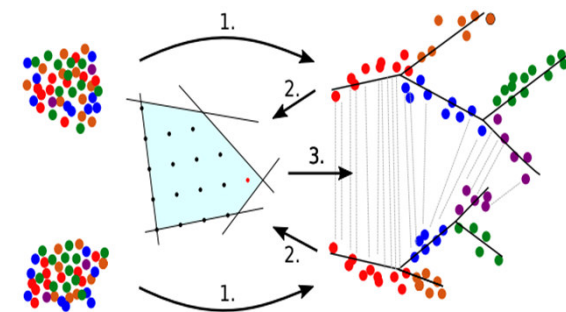
Do et al., Genome Biology 2021

Big data subsampling



Do et al., iScience 2020

Trajectory alignment



Do et al., RECOMB 2019

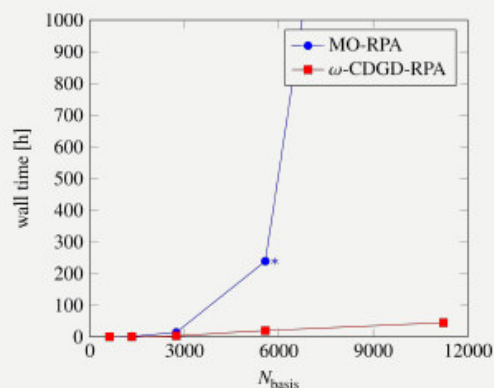
Development of Accurate and Efficient Electronic-Structure Methods



Dr. Daniel Graf
AK Prof. Ochsenfeld

- [1] *J. Chem. Theory Comput.* **14**, 2505 (2018)
- [2] *J. Chem. Phys.* **148**, 204104 (2018)
- [3] *J. Chem. Theory Comput.* **15**, 4468 (2019)
- [4] *J. Chem. Theory Comput.* **16**, 2985 (2020)
- [5] *J. Chem. Theory Comput.* **16**, 6856 (2020)
- [6] *J. Chem. Phys.* **153**, 244118 (2020)
- [7] *J. Chem. Theory Comput.* **17**, 5623 (2021)

High Efficiency:



Low Memory Requirements:

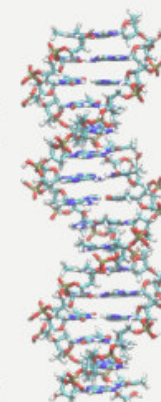
Optimized Batching

- Minimizing Overhead
- Optimizing Resource Utilization

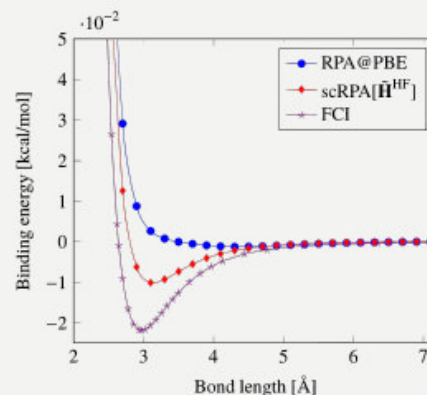


(DNA)₁₆

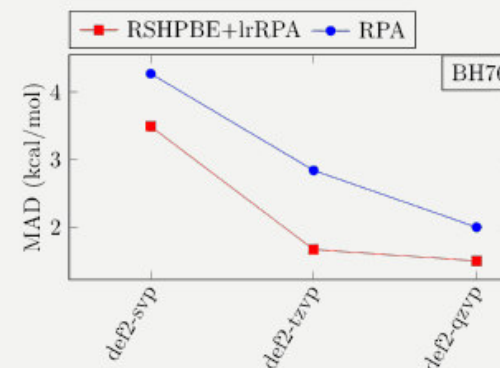
- 1052 Atoms
- 11230 Basis Func.
- 12 TB → 41 GB RAM



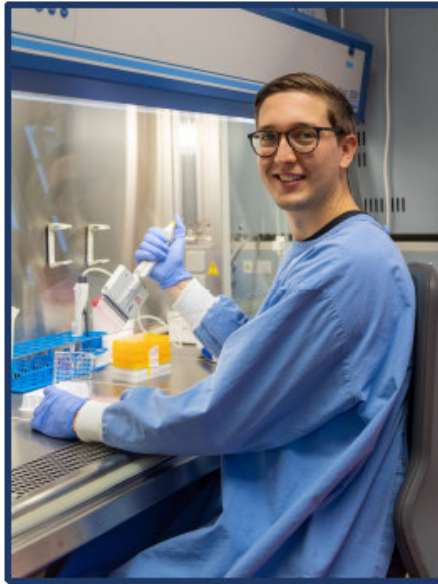
Improved Accuracy:



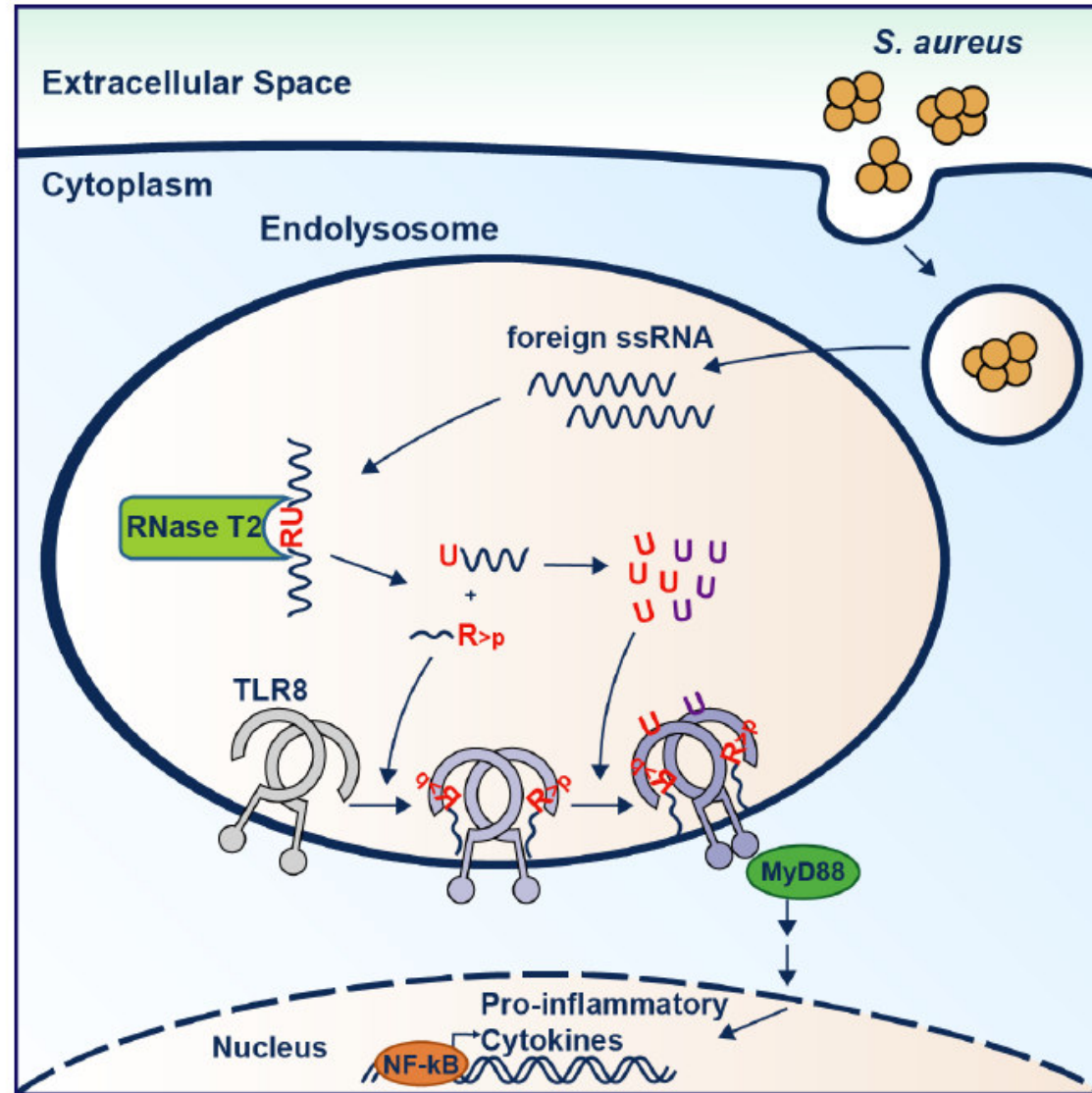
Improved Basis-Set Convergence:



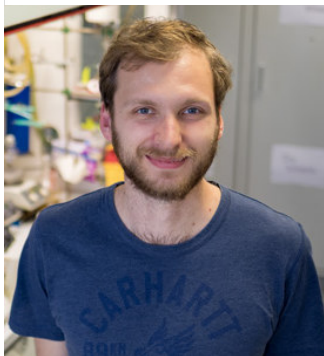
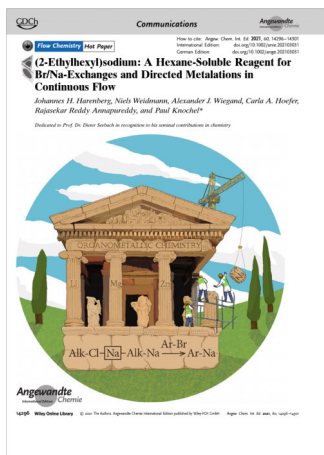
TLR8 Is a Sensor of RNase T2 Degradation Products



Dr. Wilhelm Greulich
AG Hornung
Innate Immunity

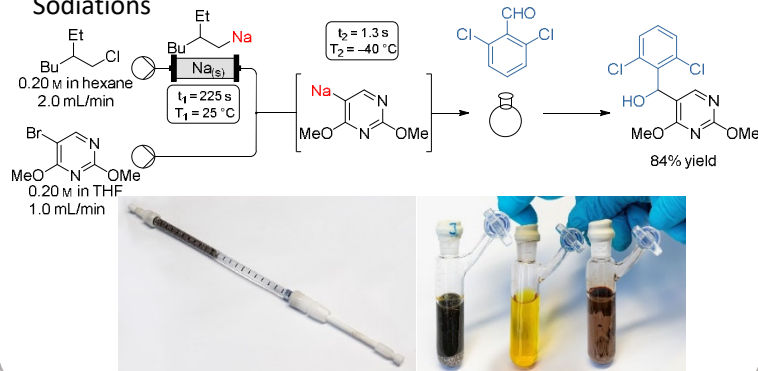


Generation and Use of Alkaliorganometallics in Continuous Flow



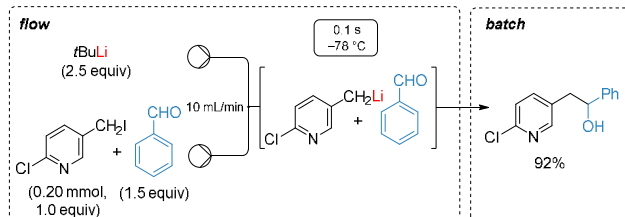
Johannes Harenberg
AK Prof. Dr. Knochel

Preparation of (2-Ethylhexyl)sodium using a Na-Packed-Bed Reactor and its use in Br/Na-Exchanges and Directed Sodiations



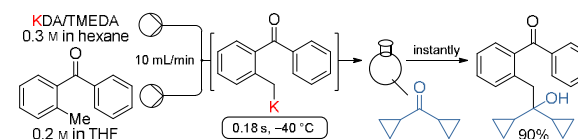
Angew. Chem. Int. Ed. **2021**, *60*, 14296 – 14301.

Preparation of Benzylic Lithium Organometallics via Br/Li-Exchange in Continuous Flow



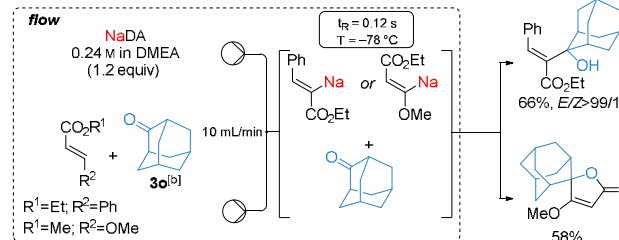
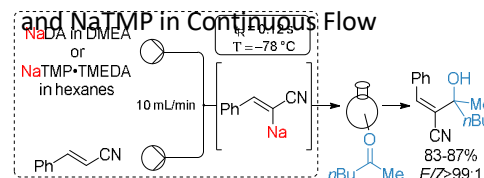
Org. Lett. **2020**, *22*, 5895 – 5899.

Preparation of (Hetero)aryl and Benzylic Potassium Organometallics using KDA in Continuous Flow



Angew. Chem. Int. Ed. **2020**, *59*, 12321 – 12325.

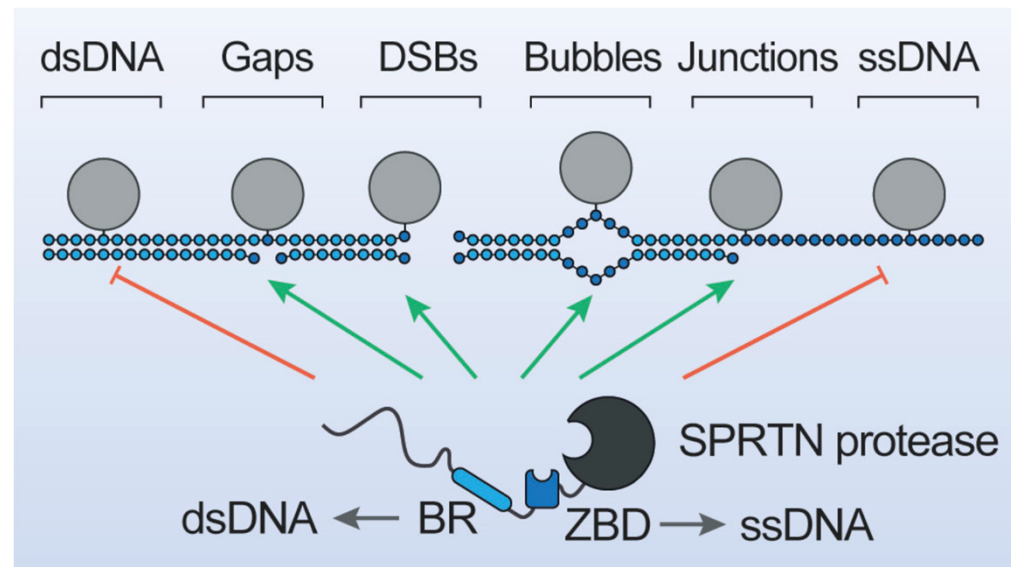
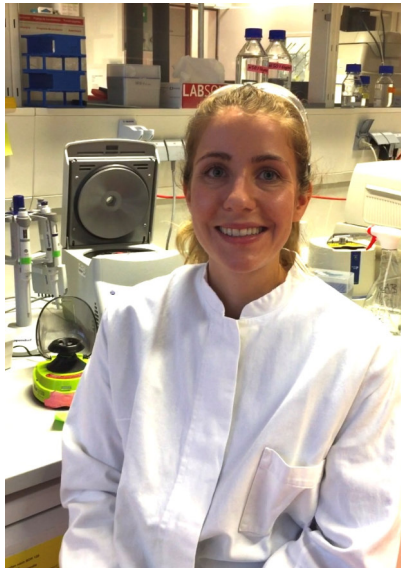
Sodiation of Acrylates and Acrylonitriles using NaDA



Angew. Chem. Int. Ed. **2021**, *60*, 731 – 735.

DNA-protein crosslink repair by the SPRTN protease

Hannah Reinking
AG Stinglele



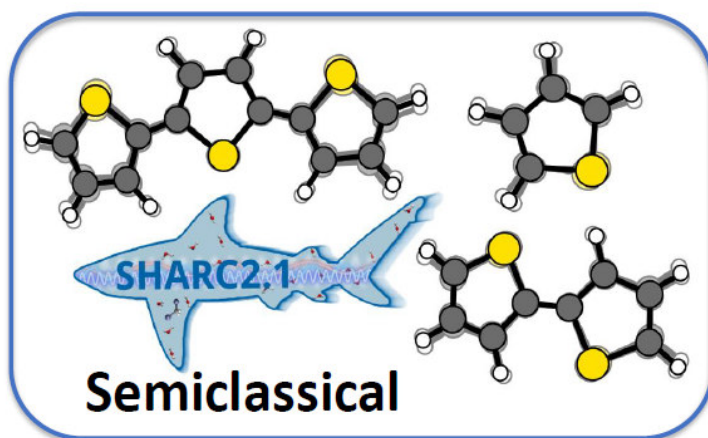
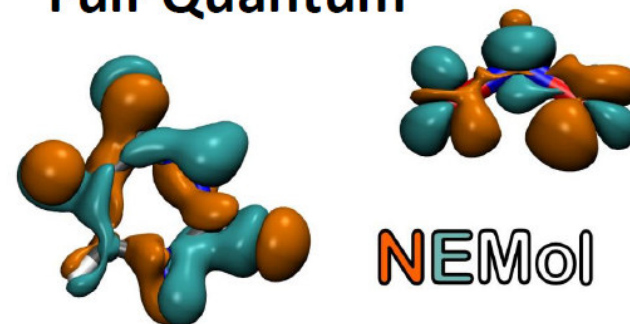
Römer-Preis auf dem Gebiet der Biochemie

Coupled Nuclear and Electron Dynamics in Molecules: From Semiclassical to Full-Quantum

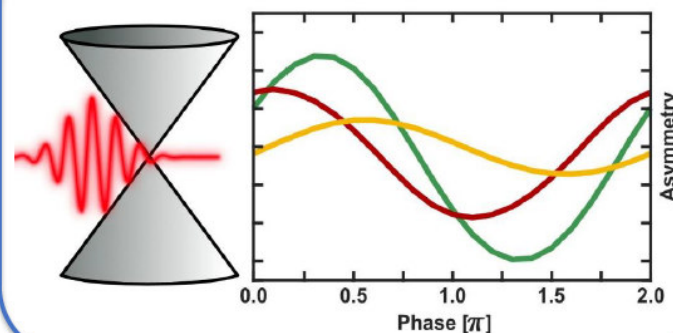


Dr. Thomas Schnappinger
Theoretical Femtosience
AK de Vivie-Riedle

Full-Quantum

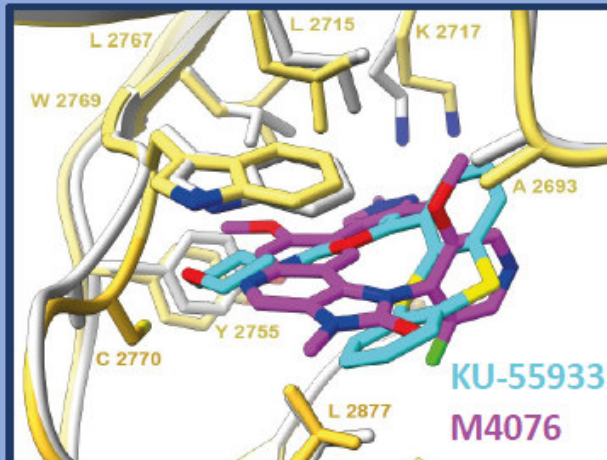
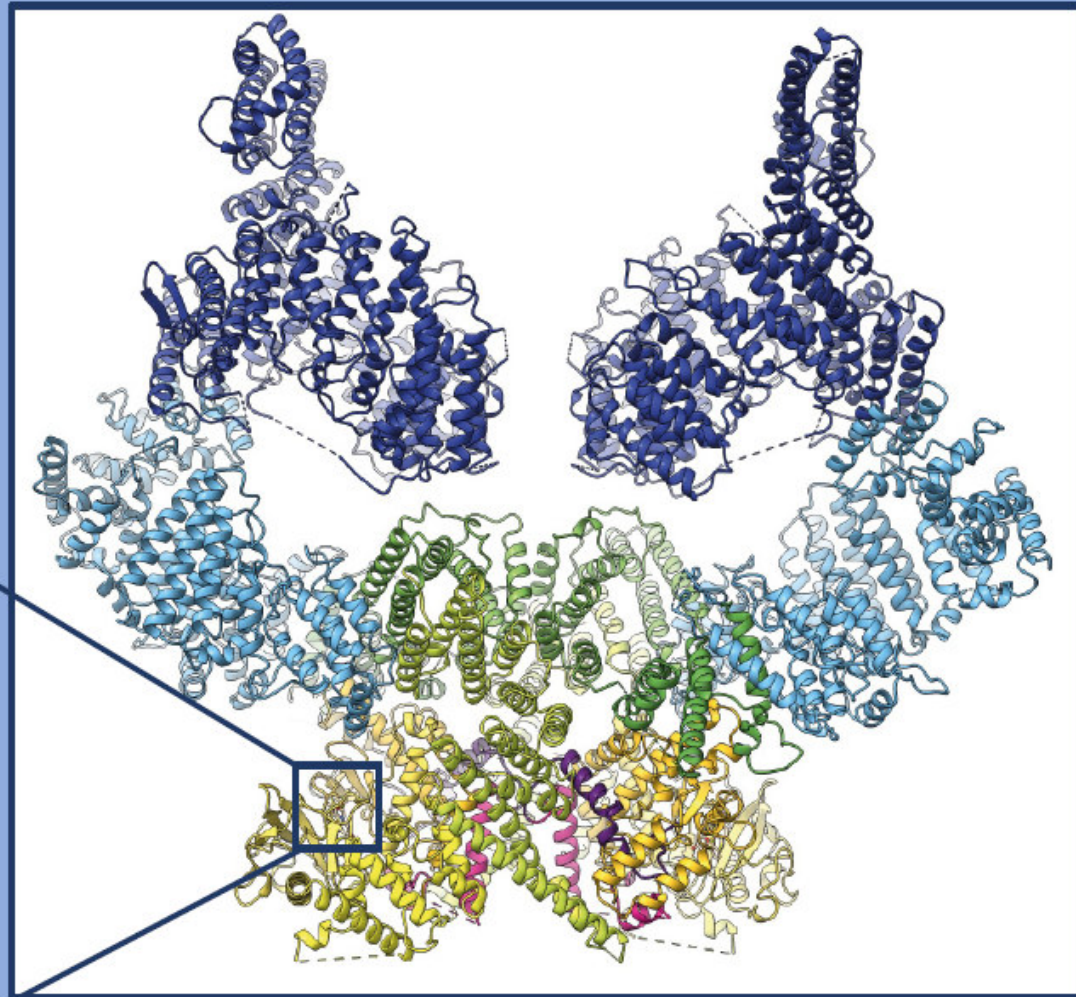
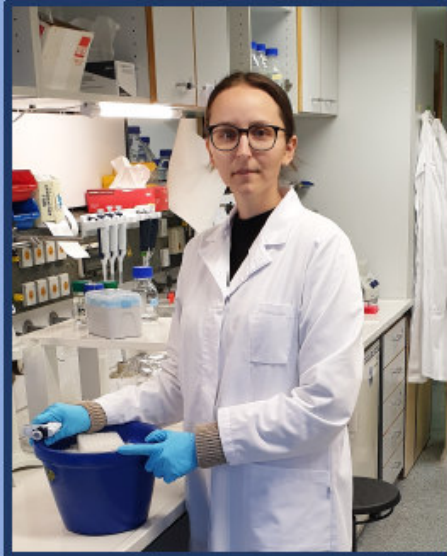


Control

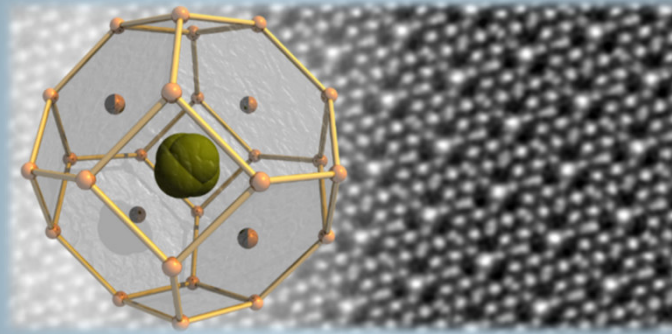


Kristina Stakyte
AG Hopfner

DNA damage repair
Molecular basis of human ATM kinase inhibition



Inhibitors bound in the active site of human ATM

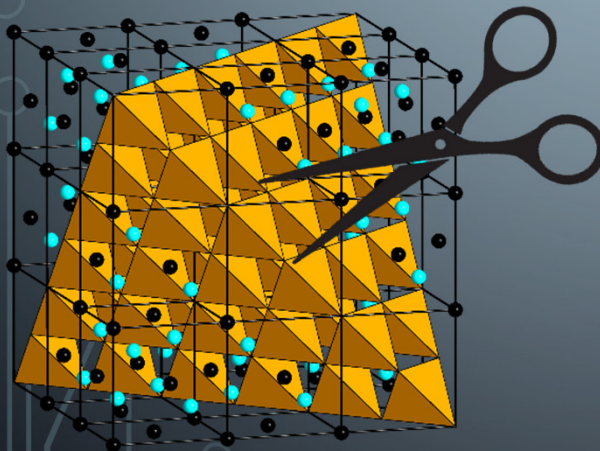


neuartige halbleitende Sodalithe

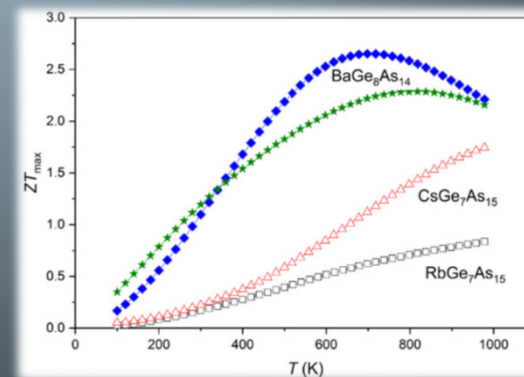


Anorganische Festkörperchemie - Grundlagenforschung im Bereich der Halbleiter und Thermoelektrik

GaAs basierte Supertetraeder



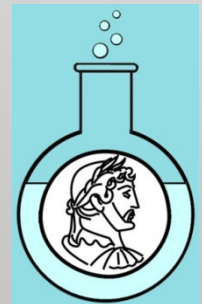
High Performance Thermoelektrika



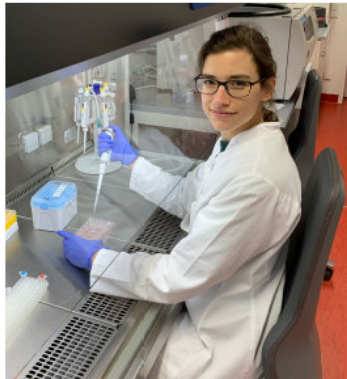
Valentin Weippert
AK Johrendt

Mit 5.000 € dotierte PostDoc-Preise für
exzellente Leistungen erhielten

Dr. Evelyn Fessler
Dr. Viktorija
Glembockyte



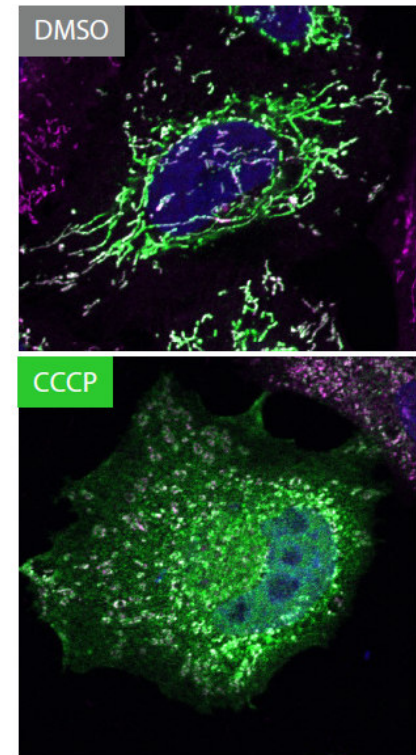
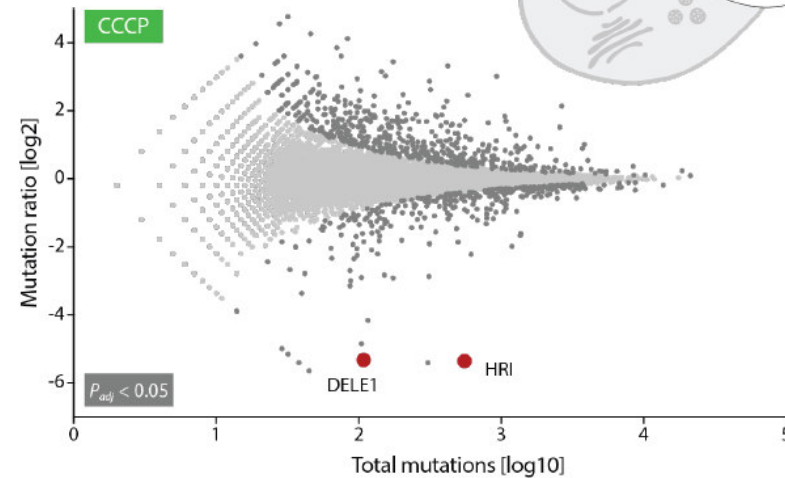
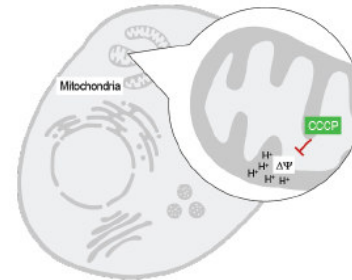
Dissecting mito-nuclear stress signaling using haploid genetics



Evelyn Fessler
AG Jae
Functional Genomics



How do mitochondria handle stress?



DELE1 | mitochondria | nuclei

Römer-Preis 2021 in der Kategorie PostDocs



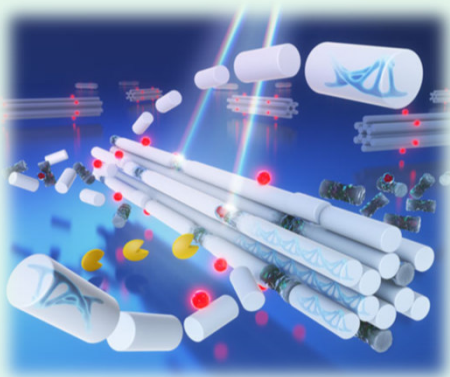
**Dr. Viktorija
Glembockyte**

Marie Curie
Research Fellow

AK Tinnefeld

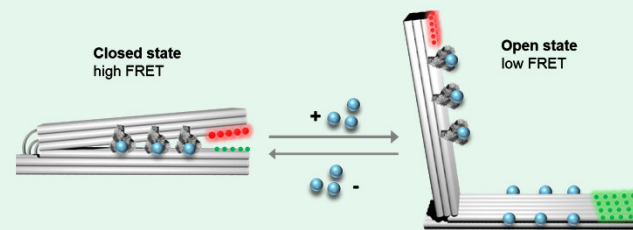
DNA origami and single-molecule imaging tools for biosensing and studying processes on the nanoscale

Self-repair and self-regeneration in DNA nanostructures

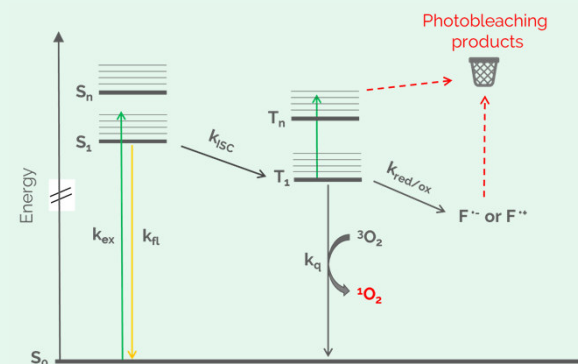


Angew. Chem. Int. Ed. 2021, 60, 4931

Building tunable and modular single molecule sensors

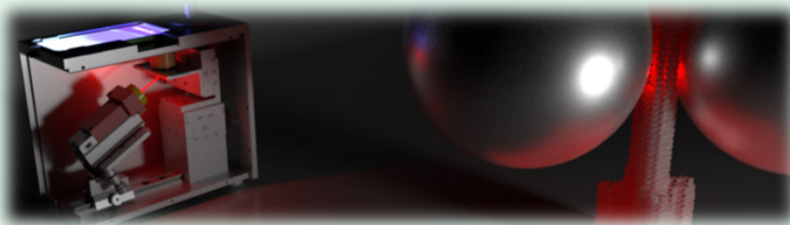


Photophysics and photostability of single molecules



Angew. Chem. Int. Ed. 2021, doi: 10.1002/anie.202109749
Meth. Appl. Fluoresc. 2020, 8, 024003
J. Phys. Chem. Lett. 2020, 11, 4462
J. Org. Chem. 2020, 85, 5907

Signal amplification strategies to detect single-molecules on the smartphone camera



Nat. Commun. 2021, 12, 950; iScience 2021, 24, 10302; Acc. Chem. Res. 2021, 54, 3338

Die Römer-Stiftung sowie
die Dozenten und Dozentinnen der
Departments Chemie und Biochemie
gratulieren den Preisträgern und
Preisträgerinnen herzlich!