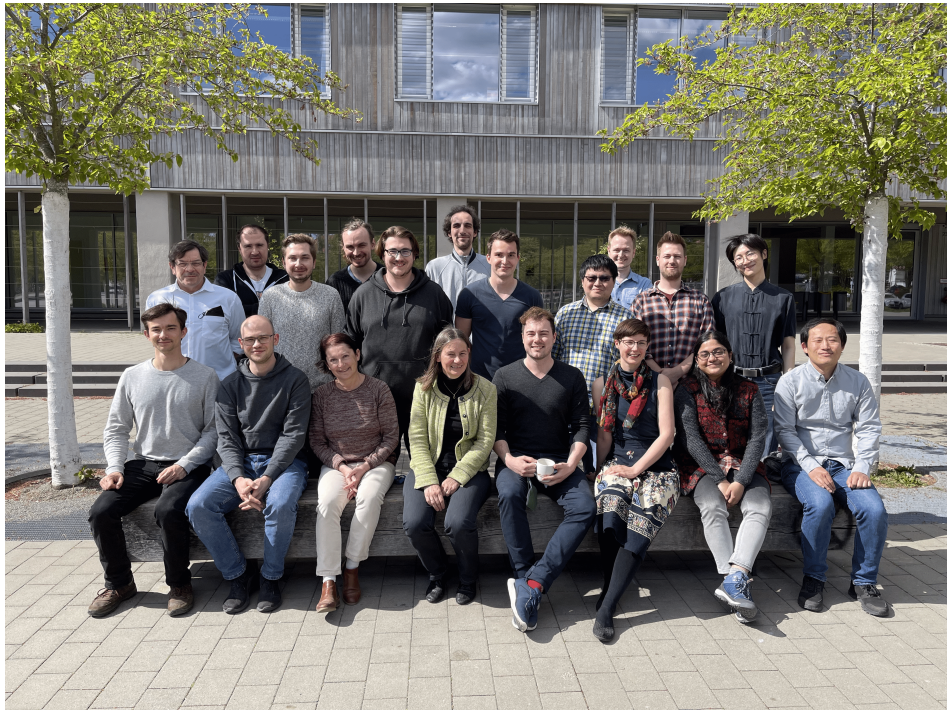

AG Paulus

Theoretical Chemistry - Quantum Chemistry

Beate Paulus, Arnimallee 22, room A224, b.paulus@fu-berlin.de

FU Berlin, 14.11.2024

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1 Research in AG Paulus

Investigating the electronic structure of molecular and periodic systems

- surface chemistry, adsorption, heterogeneous catalysis,
- material properties of various solid and surface phases
- fluorine-based catalysis
- modelling reaction pathways and transition states
- low dimensional structures and their interaction with molecules
- now topics are coming up regularly

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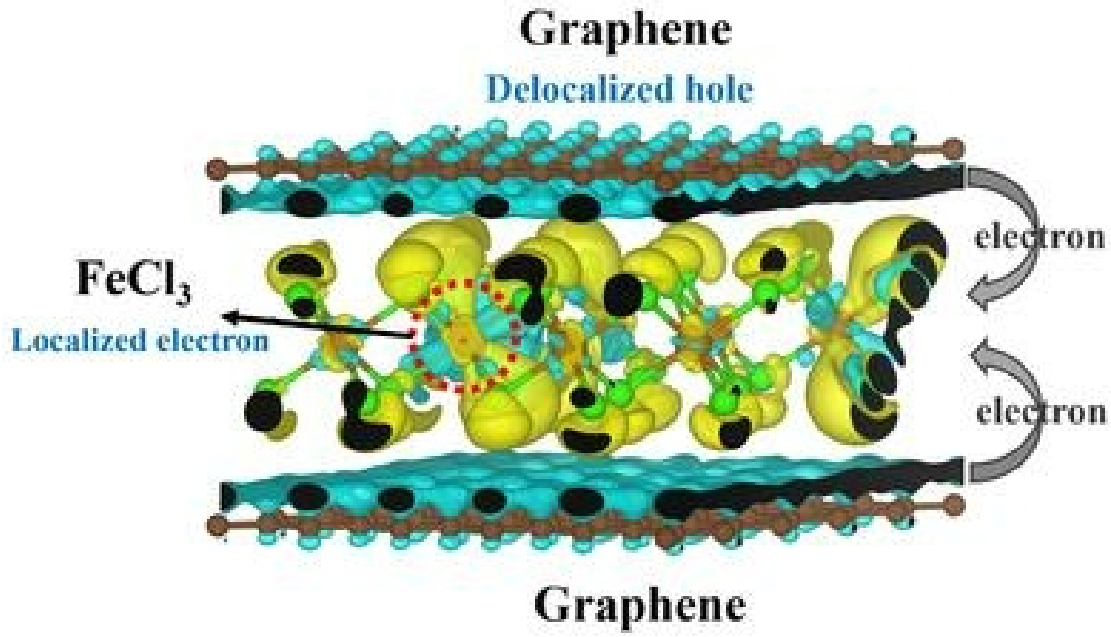
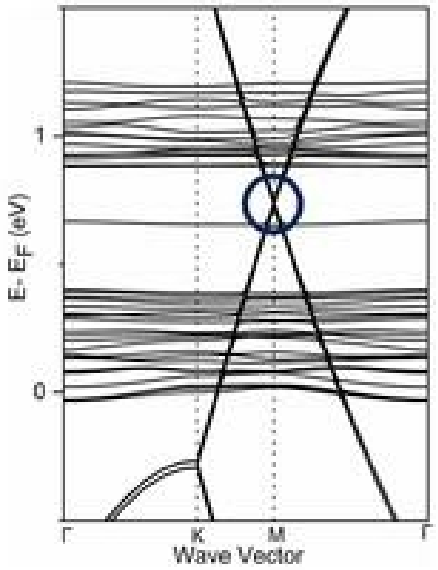
1.1 Graphitic intercalation compounds

(Dai et al., C 2023, 9(4), 95)





Band Structure

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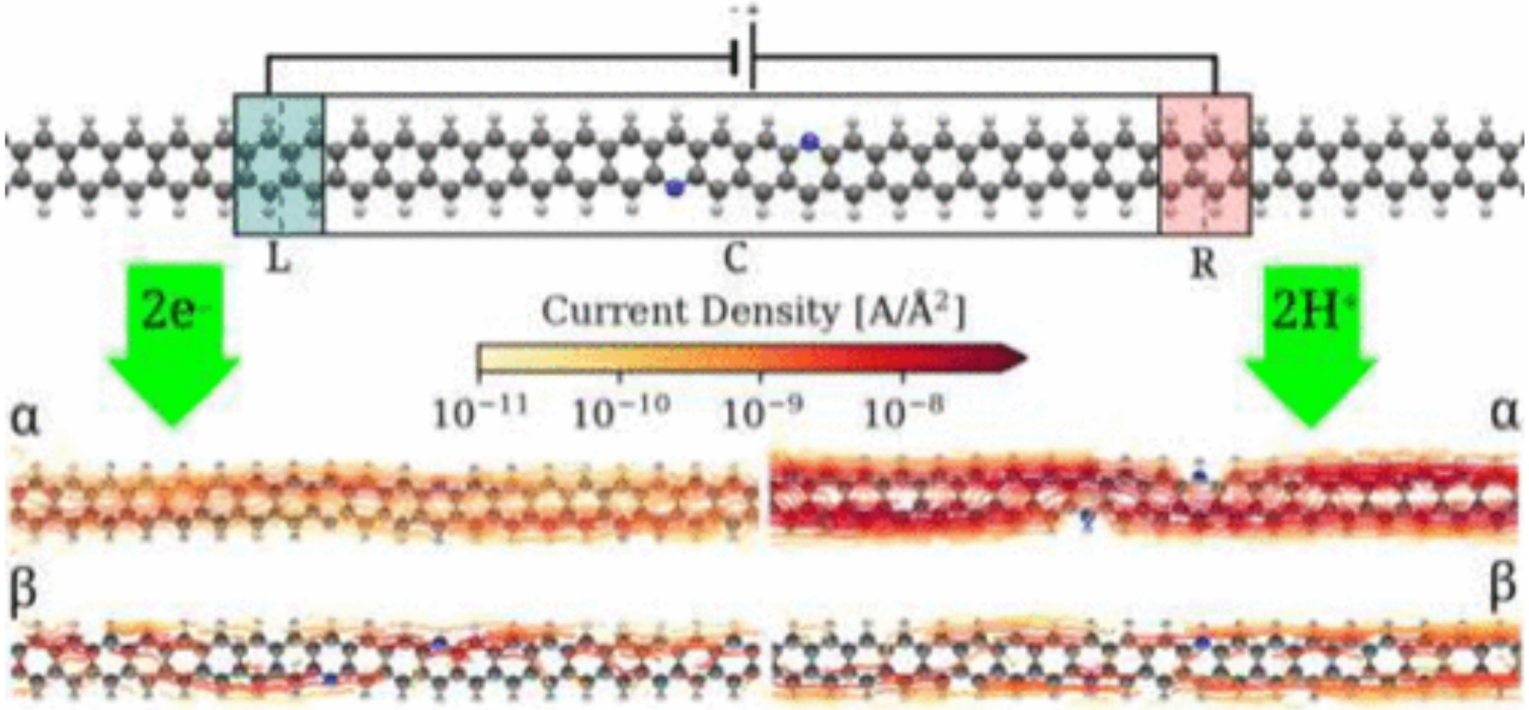
1.2 Transport in low dimensions - molecular electronics

(Conrad et al., J. Phys. Chem. C 2024, 128(44), 18886-18893)



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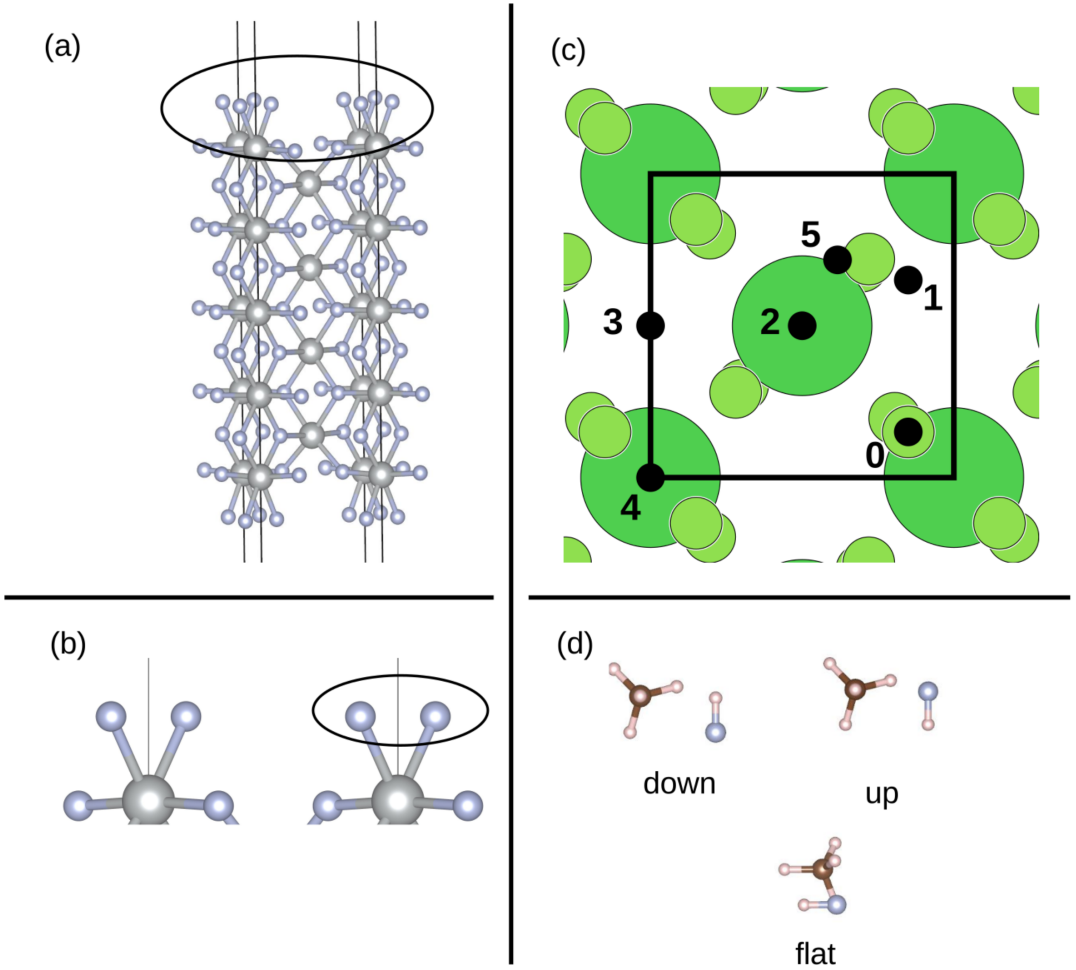
1.3 Catalysis in Nickelfluorides - Simons' process

(Lindic et al., Materials 2024, 17(9), 2062)



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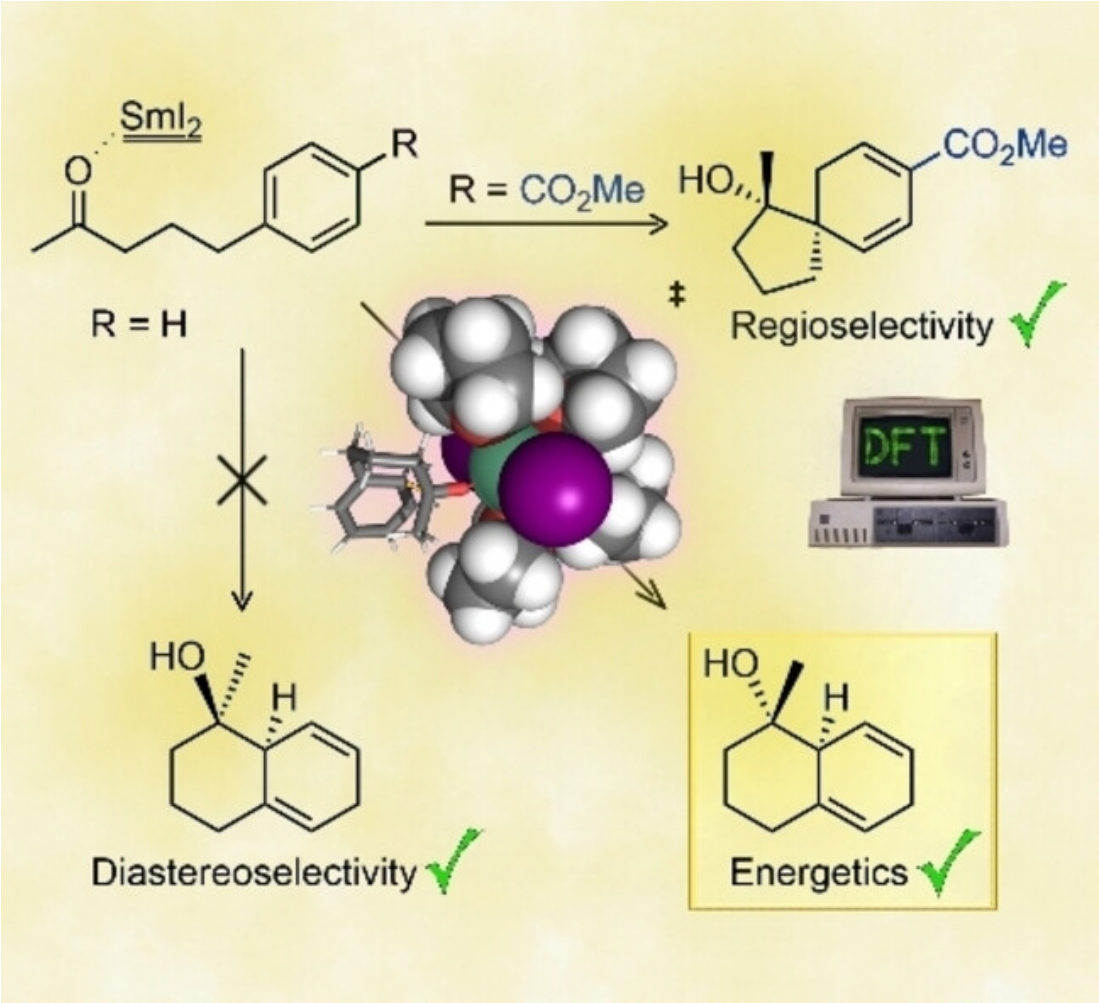
1.4 Samarium diiodide promoted reactions

(Steiner et al., Chem. Eur. J. 2024, 30, e202401120)



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2 How to apply for research work in AG Paulus

- prerequisite: Quantum chemistry course
- per email to b.paulus@fu-berlin.de ...
  - what you want to do?
  - when you want to start?
  - interest in research field
- about 2 month before you would like to start
- possibility to support research outside the institute if it fits topic-wise

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3 Independent research groups in theoretical chemistry

- Dr. Denis Artiukhin: Proton-coupled electron tranfer reactions
  method and code development
  poster today; contact: den@zedat.fu-berlin.de
- Dr. Jan Philipp Götze: Quantum Chemistry for biosystems
  photochemistry in biosystems, QM/MM methods, method and code development
  contact: jgoetze@zedat.fu-berlin.de
- PD Dr. Dirk Andrae: Highly accurate quantum chemistry for small systems
  multi-reference methods, relativistic effects, benchmarking
  contact: dirk.andrae@fu-berlin.de

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4 What you can learn additionally

- Linux and high performance computing
- Latex
- transfer of QC results to experimental chemists
- programming
- handling large data
- work in an international environment