TECHNISCHE UNIVERSITÄT DRESDEN

CRC 1415

complex nano materials

DRESDEN concept

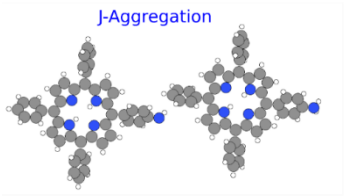
Chair of Materials Science and Nanotechnology

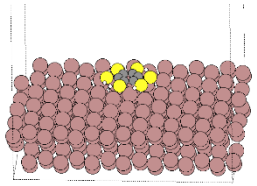
Rational Design of 2D Polymers

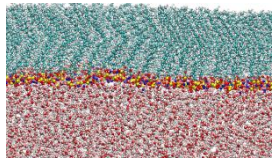
2nd TAC Meeting // 30.08.2022

David Bodesheim

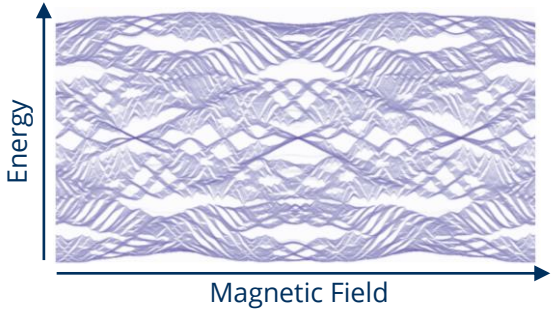
Rational Design of 2D Polymers



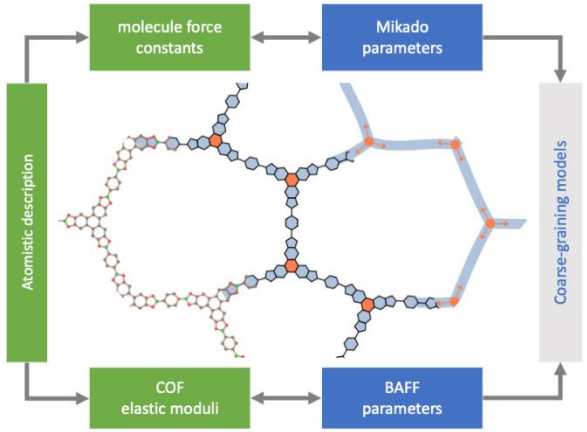


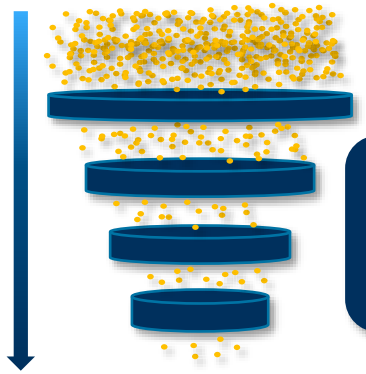


Elucidating the Synthesis of 2D Polymers at Interfaces



Electronic and Elastic Properties





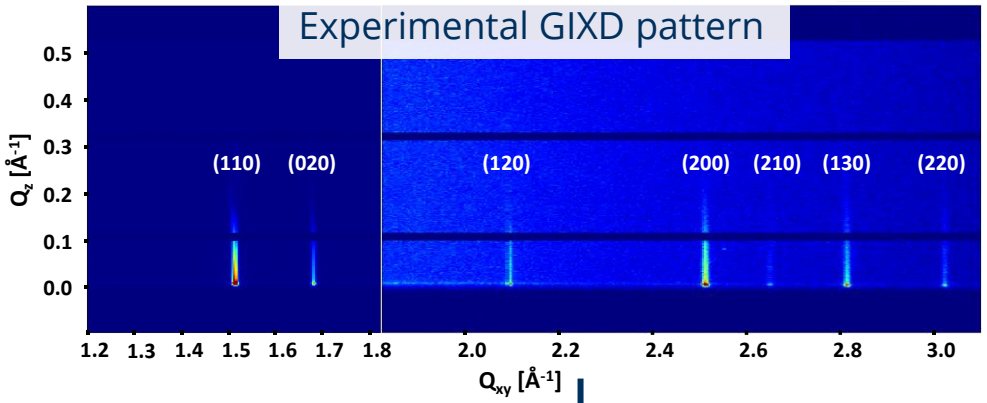
High-Throughput Calculations

Elucidating the Synthesis of 2D Polymers at Interfaces

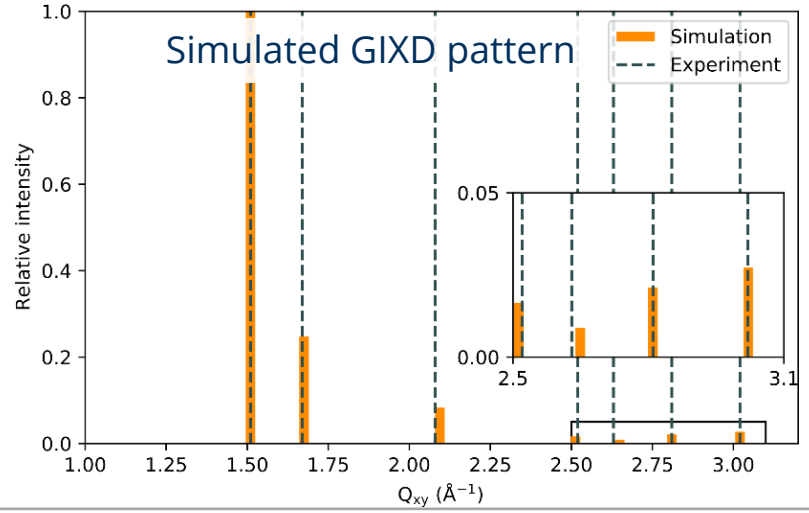
In preparation

Anupam Prasoon
(Dr. Renhao Dong)

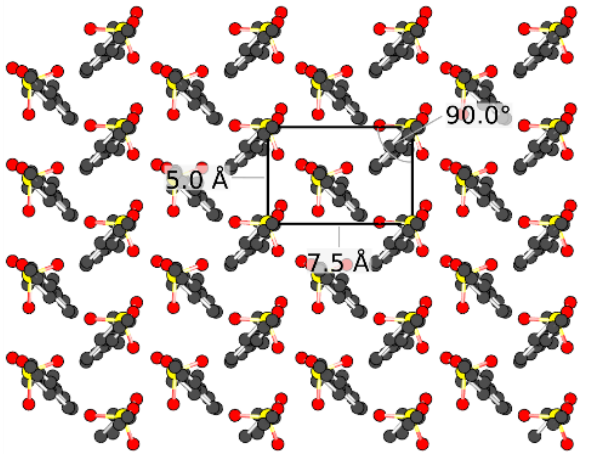
Packing of surfactants at water interface



Basic scattering theory



SOS packing (top view)



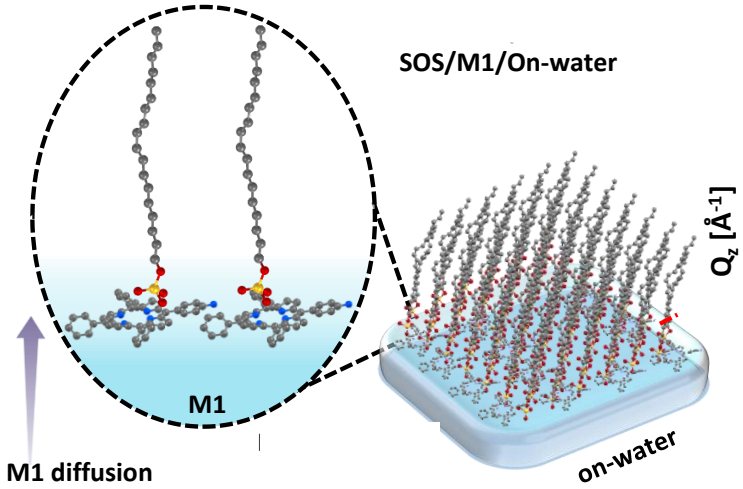
Elucidating the Synthesis of 2D Polymers at Interfaces

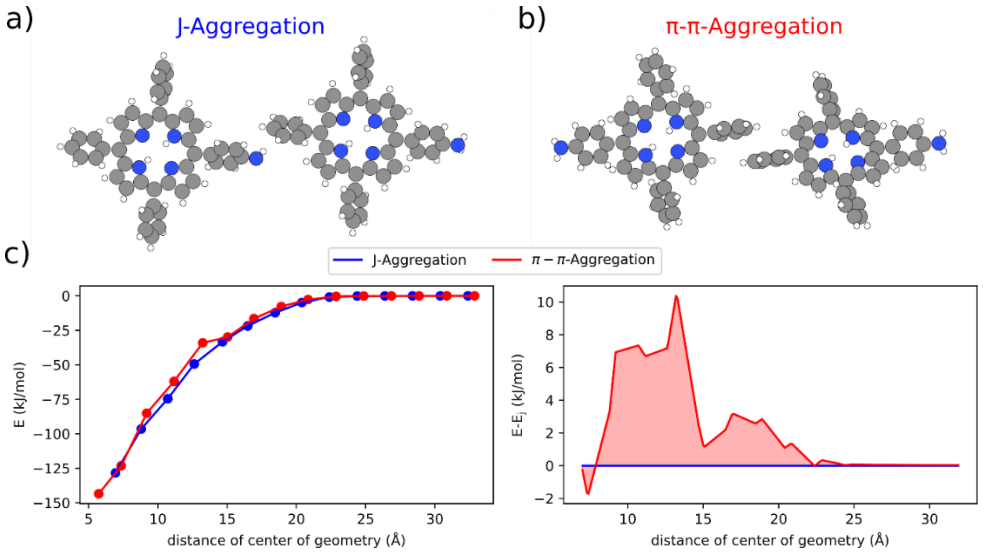
In preparation

Anupam Prasoon
(Dr. Renhao Dong)

Pre-Assembly of monomers at water-surfactant interface

Hypothesis that J-Aggregated structure is predominant supported by DFTB calculations

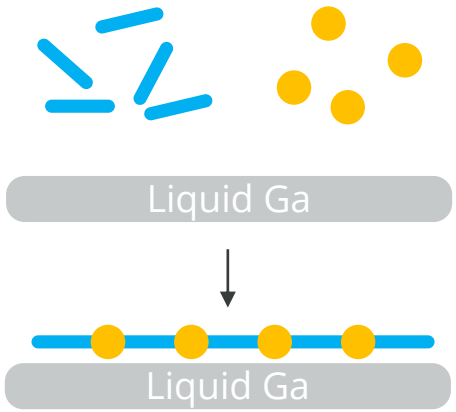


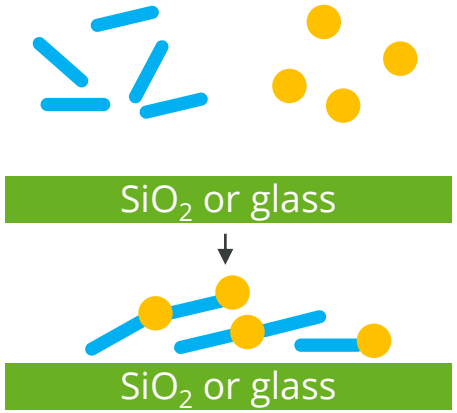


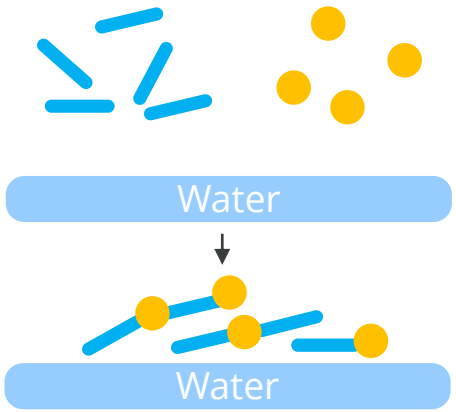
Furthermore, IR/Raman calculations to verify experimental spectra of monomer assembly at surface.

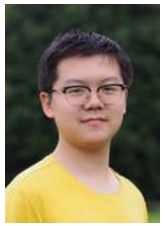
Elucidating the Synthesis of 2D Polymers at Interfaces

2D Polymer Synthesis on liquid Gallium

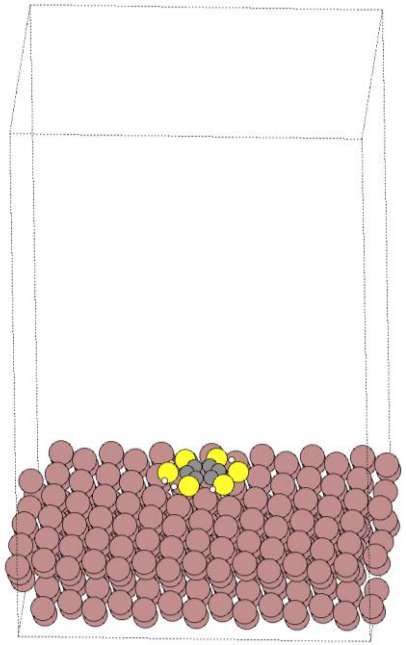


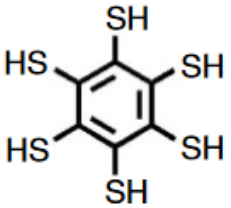






Dr. Jinxin Liu
(Dr. Renhao Dong)



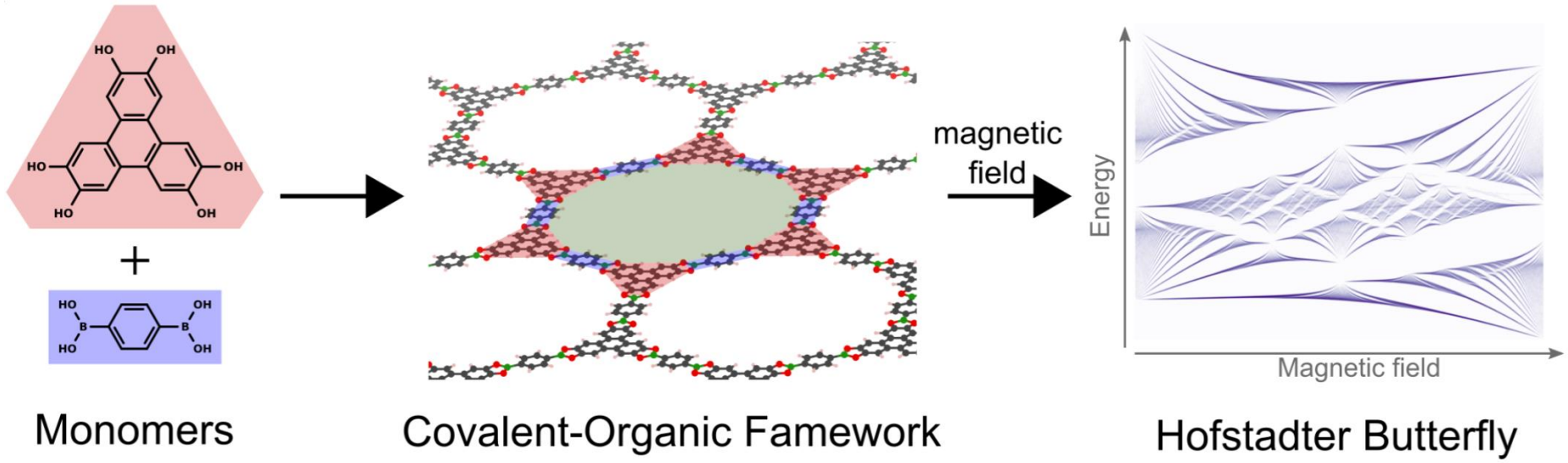


Calculation of
Adsorption Energies

Electronic and Elastic Properties

Under Review

Hofstader Butterfly in 2D COFs

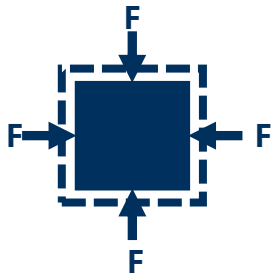


Electronic and Elastic Properties

arXiv:2207.06787

Coarse-Graining Elasticity in 2D COFs

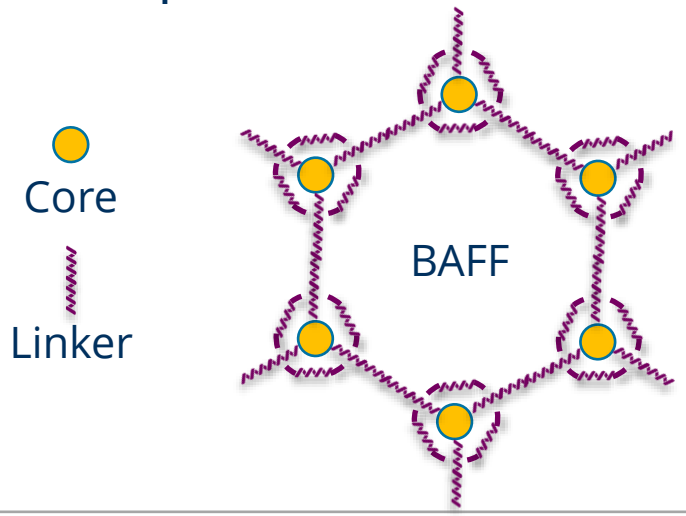
2D Bulk Modulus

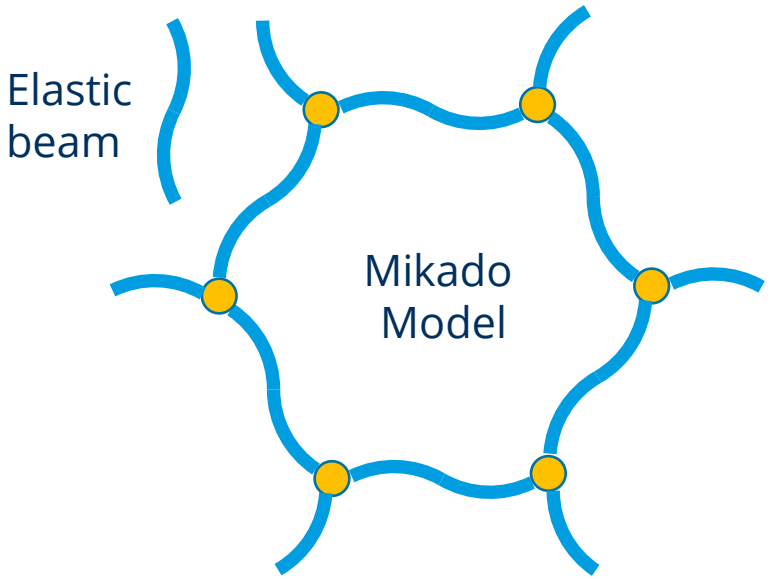


2D Shear Modulus

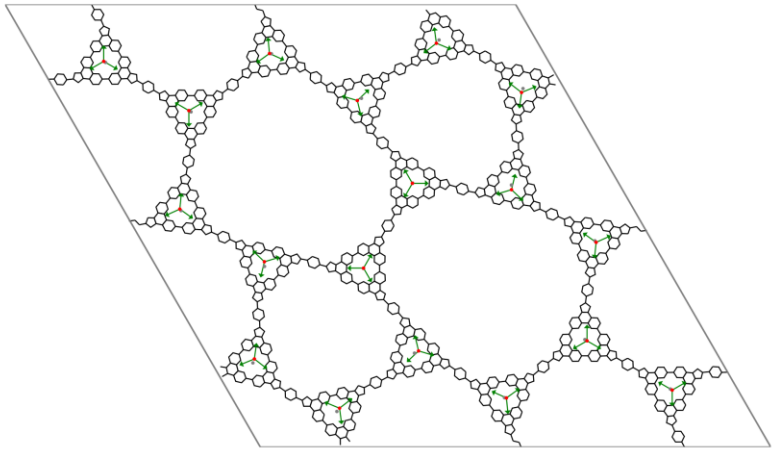
Stretching Linker

Bending Linker





Coarse-Graining for larger scales
Example: Defects



High-Throughput Calculations

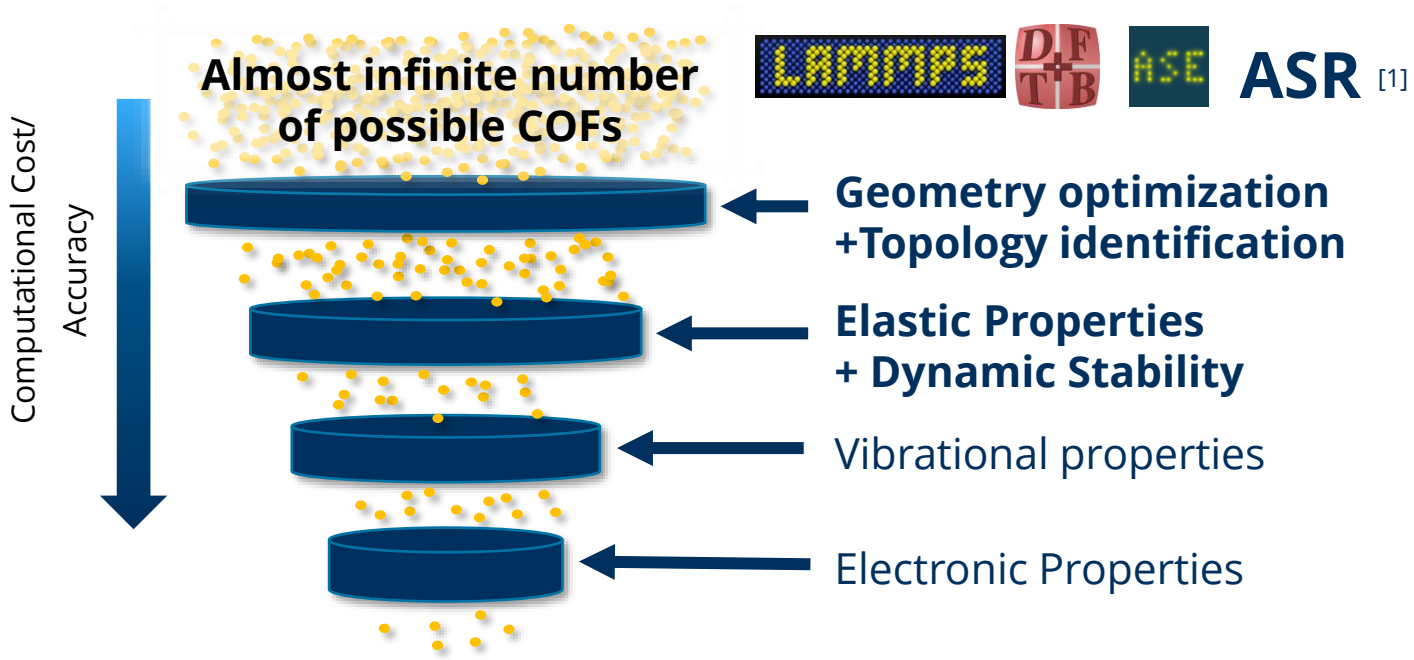
Numbers from some existing COF-Databases…

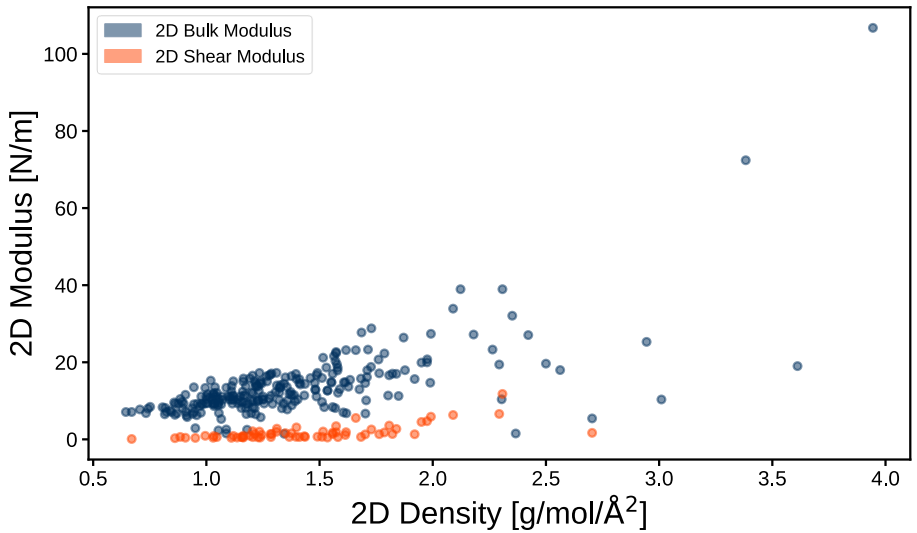
J. Phys. Chem. C 2018, 122, 24, 13009–13016: **811**

Chem. Mater. 2018, 30, 15, 5069–5086: **69,840**

Nat. Comm. 9, 5274 (2018): **470,000**

→ Screening must be **efficient** and **scalable**!



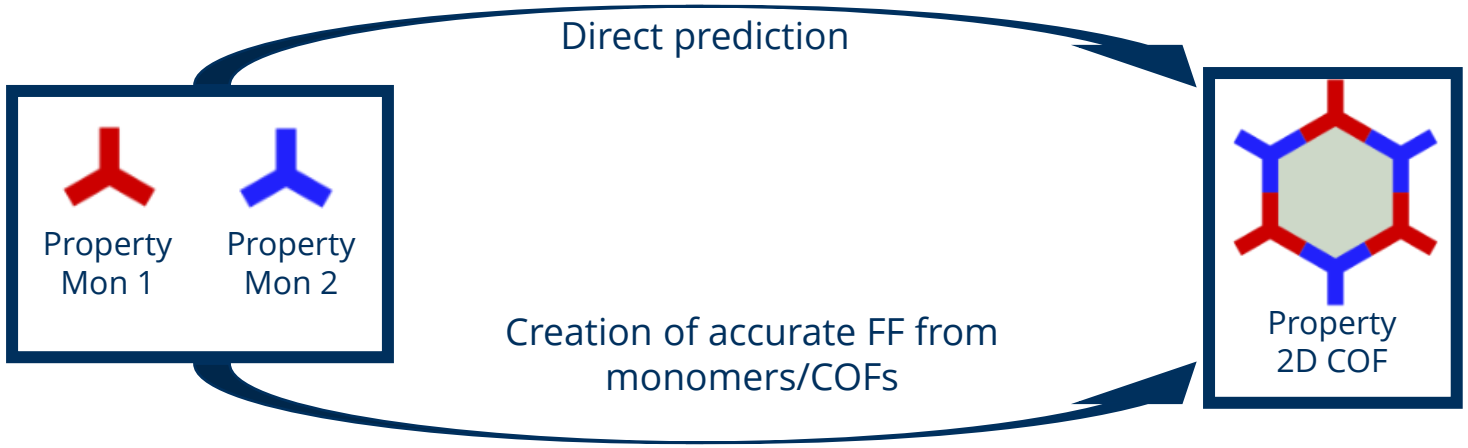


[1] Computational materials science, 199, 110731 (2021)

High-Throughput Calculations

From monomer properties to COF properties

Work in progress of decomposition algorithm of COFs to molecules



Other activities

Supervision of Master/Diploma Students

- Siddhant Biswas
  Tight-Binding in 2D COFs
  (External)

- Jonathan Heinze
  High-Throughput Calculations

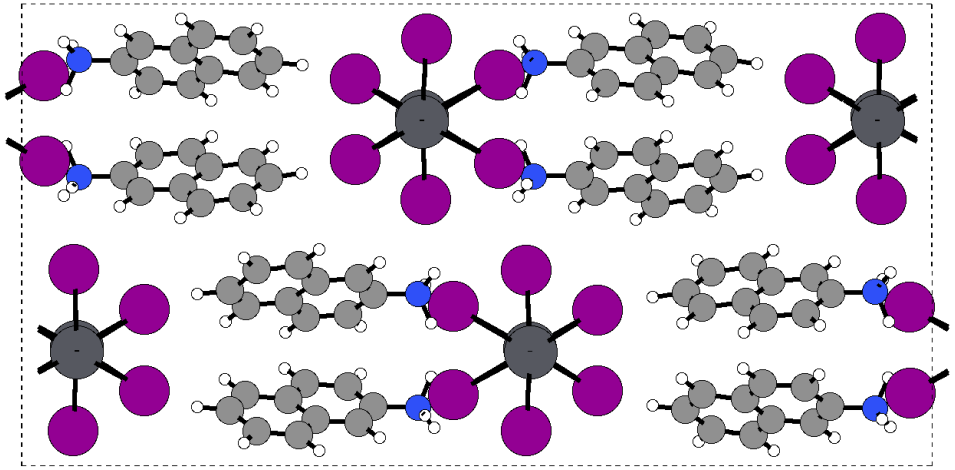
- Li Chen
  2D Sensor Materials for Odor Molecules

Helping Solving Crystal Structure of low-dimensional Perovskites

In preparation

Collaboration with Prof. Brigitte Voit and Dr. Agnieszka Kuc

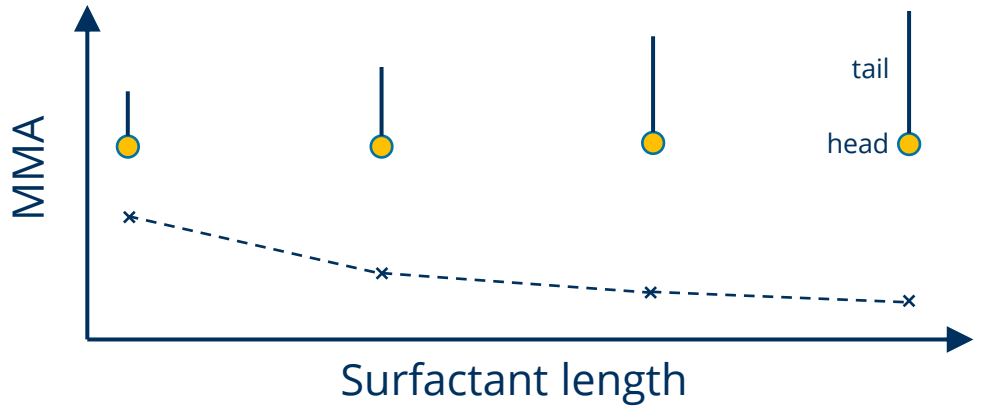
Andrei Mitrofanov



Outlook

In General: Finishing up started projects!

More work on surfactants
- Relationship of surfactant-type and density of packing/electrostatic potential
- Diffusion of Monomer towards surfactants



High-Throughput Calculations
- Scaling up workflow
- Implementing features like:
  - Electronic structure (Band structure, Band gap, etc.)
  - pXRD patterns
  - IR/Raman
  - …
- Sharing with public ➔ help for CRC

Coarse-Graining for COFs
- Generalizing Coarse-Graining approach
- Application to defective systems

Other details

Conferences in 2022:

APS March Meeting, Chicago

Psi-K, Lausanne

DPG Frühjahrstagung, Regensburg

Summer Schools:

DFTB+ Summer School, Daresbury

Vorgezogenes Rigorosum:

Nanostructured Materials

Transport properties of emergent materials in solid state physics (Prof. Helena Reichlova)