







Chair of Materials Science and Nanotechnology

# **Rational Design of 2D Polymers**

TAC Meeting // 14.02.2024 David Bodesheim



Elucidating the Synthesis of 2D Polymers at Interfaces





# Rational Design of 2D Polymers



Electronic and Elastic Properties



High-Throughput Calculations



Control of Crystallinity of Vinylene-Linked Two-Dimensional Conjugated Polymers by Rational Monomer Design



• Calculation of reaction barriers

D. L. Pastoetter, **D. Bodesheim**, G. Cuniberti, X. Feng, et al. *Chemistry A European J.* **2022**, 28, e202104502.

### Toward Coarse-Grained Elasticity of Single-Layer Covalent Organic Frameworks



- Elasticity calculations via DFTB
- Co-Development of methods

A. Croy, A. Raptakis, **D. Bodesheim**, A. Dianat, G. Cuniberti, *J. Phys. Chem. C* **2022**, 126, 18943–18951.







Molecular engineering of naphthalene spacers in low-dimensional perovskites



• Elucidation of structures of some layered perovskites via DFT calculation

A. Mitrofanov, **D. Bodesheim**, G. Cuniberti, A. Kuc, B. Voit, et al. *J. Mater. Chem. C* **2023**, 11, 5024–5031. *Hierarchies of Hofstadter butterflies in 2D covalent organic frameworks.* 





Covalent-Organic Famework

Hofstadter Butterfly

Developed tight-binding model for 2D COFs
Investigated the Hofstadter Butterfly

A. Crov. A. Raptakis. **D. Bodesheim**. A. Dianat, G. Cuniberti.

A. Croy, A. Raptakis, **D. Bodesheim**, A. Dianat, G. Cuniberti, *J. Phys. Chem. C* **2022**, 126, 18943–18951.





04



# Site-selective chemical reactions by on-water surface<br/>sequential assemblyStructural Reinforcement in Mechanically Interlocked<br/>Two-Dimensional Polymers by Suppressing Interlayer



- Writing python program for simulation of 2D XRD
- Basic understanding self-assembly via DFTB calculations

A. Prasoon, **D. Bodesheim**, G. Cuniberti, Y. Nagata, S. C. B. Mannsfeld, R. Dong, M. Bonn, X. Feng, et al. *Nat. Commun.* **2023**, 14, 8313.

# Two-Dimensional Polymers by Suppressing Interlayer Sliding b MI-M2DP i

 Probing the in-plane elasticity and the slipping behaviour of the layers

3 µm

Y. Yang, A. Knapp, D. Bodesheim, G. Cuniberti, R. Dong, A. Fery, X. Feng, et al. **2024**, DOI 10.48550/ARXIV.2401.09099. (in Revision)





3 µm



3 µm

06



On-liquid-gallium surface synthesis of ultra-smooth conductive metal-organic framework thin films



- Calculating why on liquid gallium synthesis yields smooth MOF film
  - Stronger binding energy of precursor to Ga compared to SiO2

## Fracture behavior of two-dimensional imine-based



- Calculating the fracture point of a 2D polymer
- Calculating the stiffness tensor and related properties of the 2D polymer

J. Liu, **D. Bodesheim**, G. Cuniberti X. Feng , R. Dong, et al. *Nature Synthesis* (in Revision)









Unraveling the Impact of Nitrogen Doping on the Adsorption of Volatile Organic Compounds onto Graphene



• Supervision of Li

L. Chen, **D. Bodesheim**, A. Ranjbar, A. Dianat, R. Gutierrez, G. Cuniberti (in progess) Synthesis and charge-transport study of semiconducting quasi-2D polyacetylene film of record-high mobility via ring-opening polymerization of pyrrole on water surface by SMAIS method



- Elucidate Structure
- Elif: calculate bandstructure and mobility

K. Liu, E. Ünsal, **D. Bodesheim**, G. Cuniberti, et al. (in progress)





10

Loading...





• Calculating reaction barriers on water surface for different systems

H. Chen, Z. Wang, **D. Bodesheim**, A. Dianat,, G. Cuniberti, X. Feng, et al. (in progess) Reaction Barrier Study for Glaser Coupling DMAc/water mixture and Aldol condensation





• Calculating reaction barriers on water+organic solvent surface for different systems

Y. Ye, , Z. Wang, **D. Bodesheim**, A. Dianat, G. Cuniberti, X. Feng, et al. (in progress)









### Optimized Ridge-Regression Mikado model for Coarse-Graining 2D Polymers











Rational Design of 2D Framework-Materials David Bodesheim TAC Meeting // 14.02.2024

Slide 10



# **Summary Projects**



**Sum of papers at the end of the PhD:** 14







# **Teaching and Supervision activities**

## Teaching

### <u>4xNanostructured Materials:</u>

- Grading homework assignments
- Redesigning and creating new exercises

## <u>4xConcepts of Molecular Modeling (MolMod):</u>

- Teaching Tutorial classes
- Grading final Reports
- Restructuring Tutorials
- Creating four completely new tutorial classes

### (Co-)Supervision

- 1 Lab Rotation
- 1 Bachelor's
- 5 Student jobs
- 3 Diploma/Master's Thesis







# **Time Plan**





