Towards High-Throughput Calculation of Elastic Properties in Monolayer Covalent-Organic Frameworks

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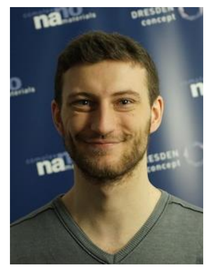
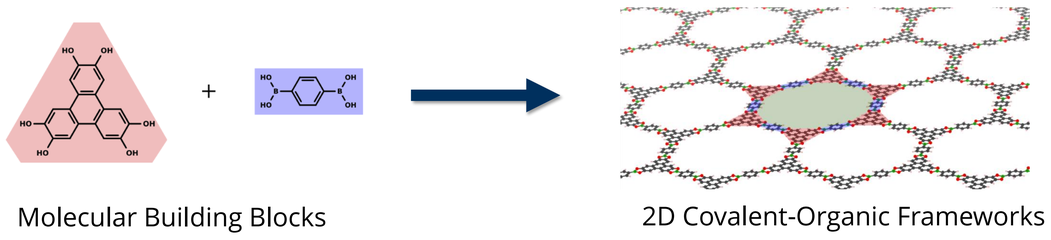
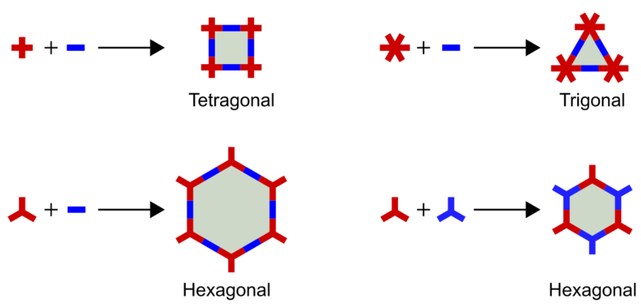


Covalent Organic Frameworks (COFs)

Due to the **combinatorial** approach of reticular chemistry, **almost infinitely many** Covalent-Organic Frameworks exist hypothetically; infeasible to verify in synthesis. Hence, we need a way too quickly and efficiently screen the COF-space for desired properties: **High-Throughput Screening**.

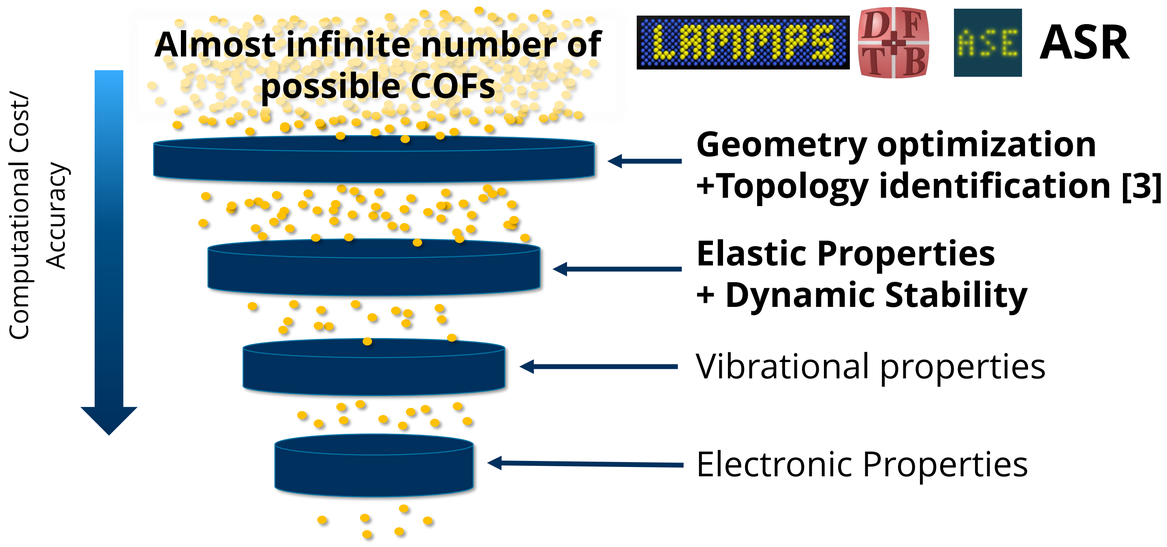


Molecule symmetries determine **Framework topologies**

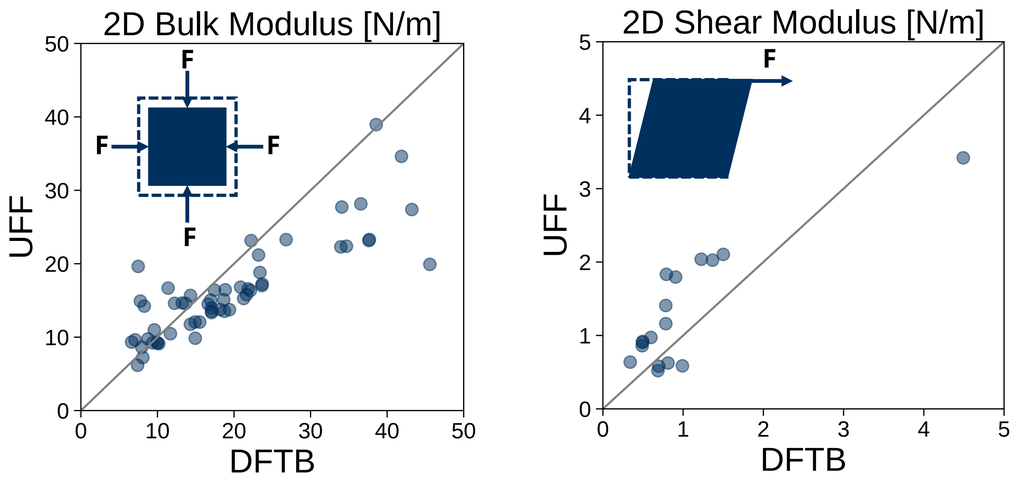


Workflow

We calculate the elastic properties of 2D COFs utilizing the **Atomic Simulation Recipes (ASR)** [1]. As ab-initio calculations for COFs are very demanding, we test if simple Force-Fields like the Universal-Force Field (**UFF**) [2] are good enough and compare it to Density Functional based Tight-Binding (**DFTB**) calculations.

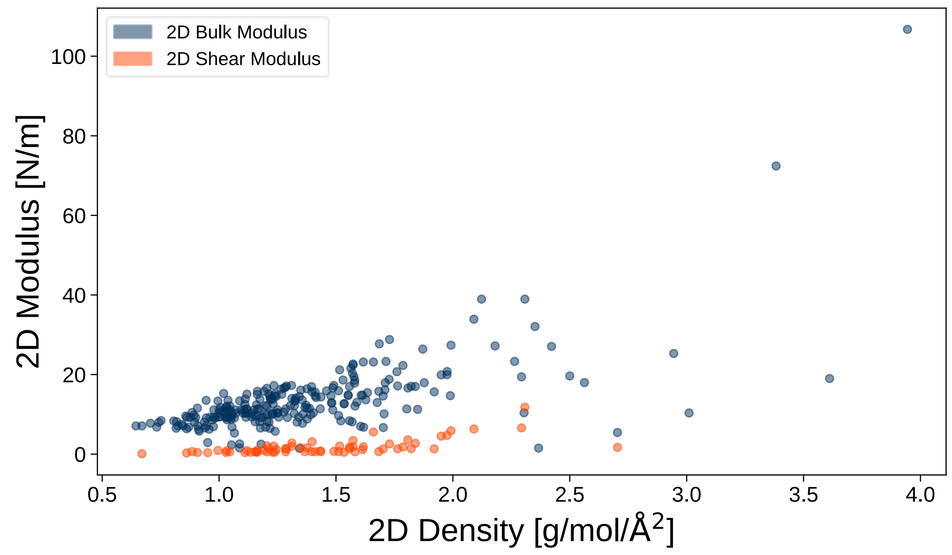


How well do simple Force Fields work?



With UFF, we can quickly determine the 2D Moduli via equation of state fitting (2D shear modulus only for hexagonal systems). Despite ist simplicity, **UFF can calculate qualitatively the correct trends in elastic properties**!

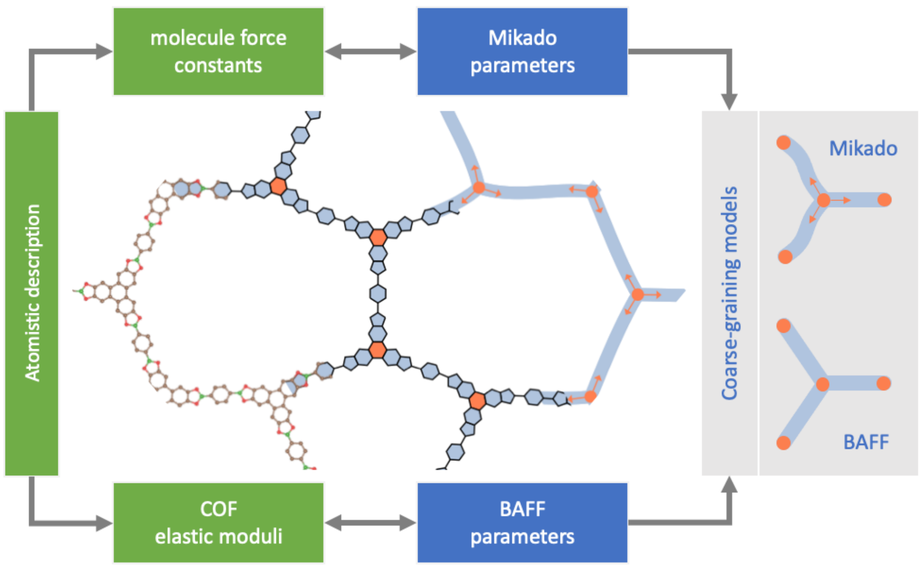
Moduli vs 2D Density (UFF)



As expected, higher 2D density correlates to higher in-plane stiffness.

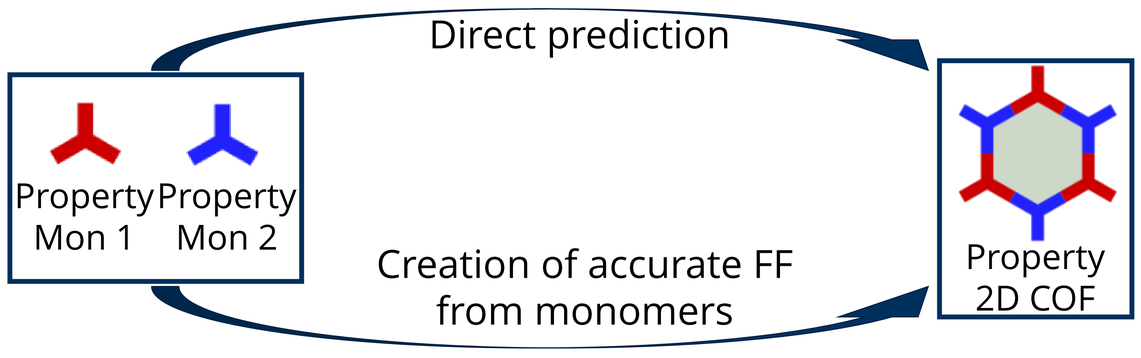
Towards Coarse-Grained Elasticity [4]

Based on the elastic moduli, we developed two coarse-grained descriptions for honeycomb COFs: A **spring network (BAFF)** and a **network of elastic beams (Mikado model)**. This allows for an efficient description of elastic deformations on larger length scales.



Outlook: From molecular to COF properties

Future plans are to apply High-Throughput calculations to bigger datasets. Furthermore, we aim to accurately predict 2D COF properties from their monomer-properties



References:

[1] Computational materials science, 199, 110731 (2021)
[2] *J. Am. Chem. Soc.* 1992, 114, 25, 10024–10035
[3] SciPost Chem. 1, 005 (2022)
[4] arXiv:2207.06787

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