chem2Dmat

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TECHNISCHE UNIVERSITÄT DRESDEN

complexnano materials

Charge Transport Characterization in Two-dimensional Covalent Organic Frameworks

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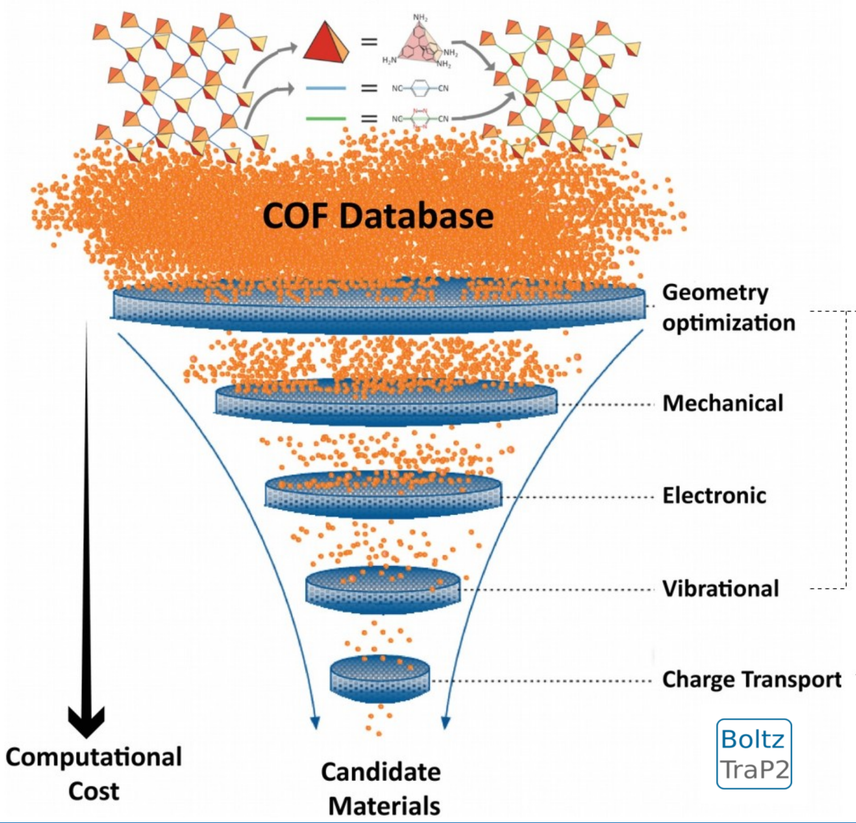
Introduction

- We investigate the charge transport properties of selected 2D COFs using a combination of atomistic approaches with Boltzmann transport theory.
- Despite the intensive studies on 2D COFs, charge transport properties of most of these materials are still unknown. In particular, their relation to molecular building block properties is a great challenge due to the combinatorial nature of reticular chemistry [1].
- Computational cost increases with the increasing complexity of the calculations.
- It is important to explore their properties systematically and to explore which material is promising.



ASE phonopy p4vasp VESTA Visualization for Electronic and STructural Analysis

DFTB VASP b-initio ienna ackage imulation QUANTUMESPRESSO

Deformation Potential Theory [2,3]

Acoustic Phonon Scattering → Constant relaxation time in 2D:

$$\tau_{acoustic} = \frac{2}{3}\frac{\hbar^3 C}{k_B T m E_d^2}$$

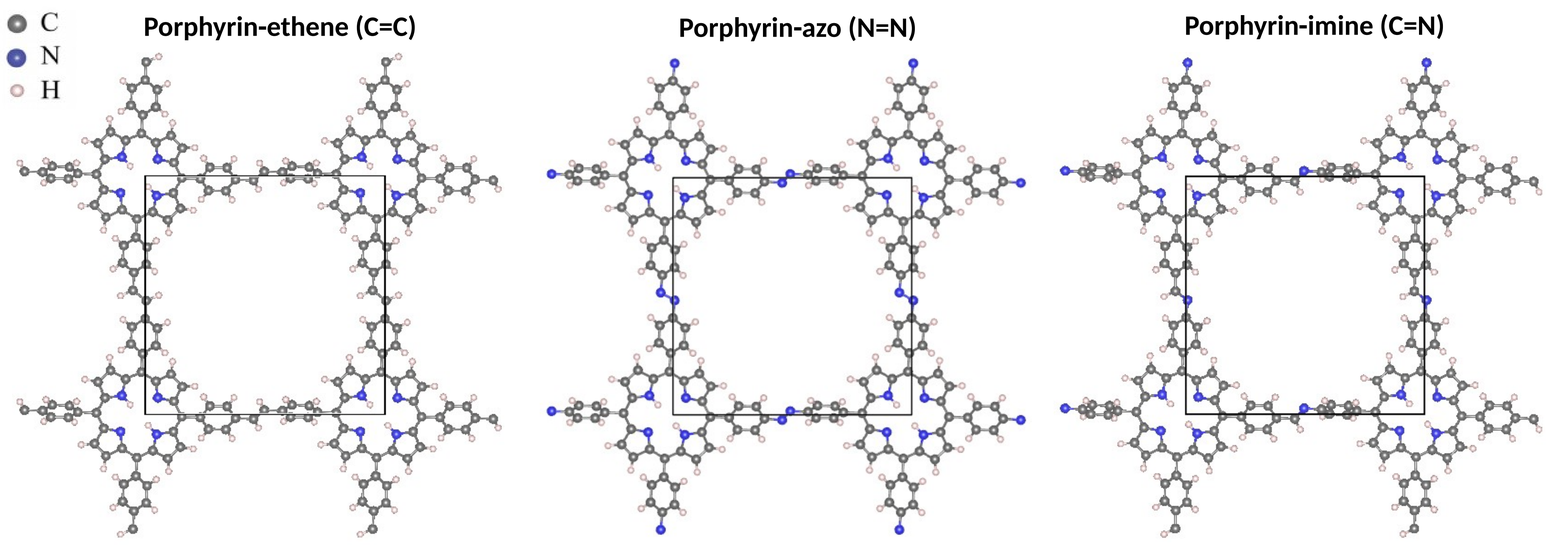
Relaxation Time Estimation

$\hbar$: Planck's constant
C : In-plane stiffness
k_B : Boltzmann constant
T : Temperature
m : Effective mass
E_d : ADP constant

Mobility

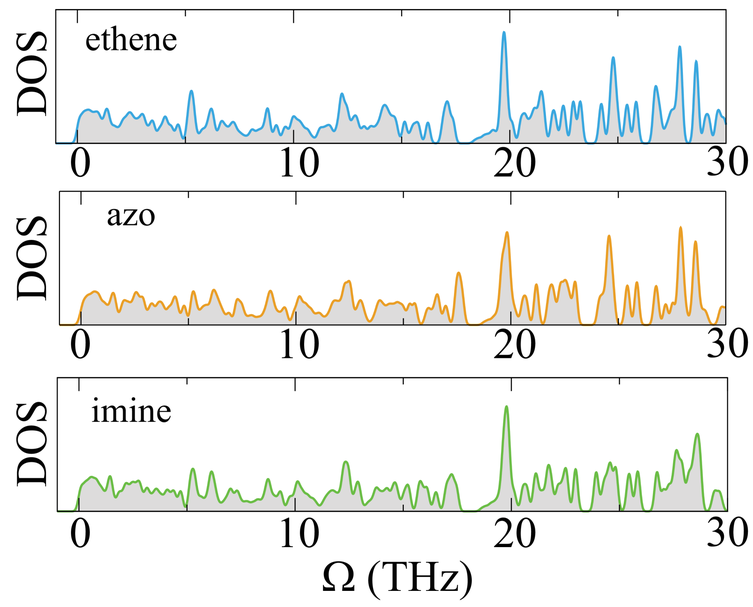
Results

Structural Properties



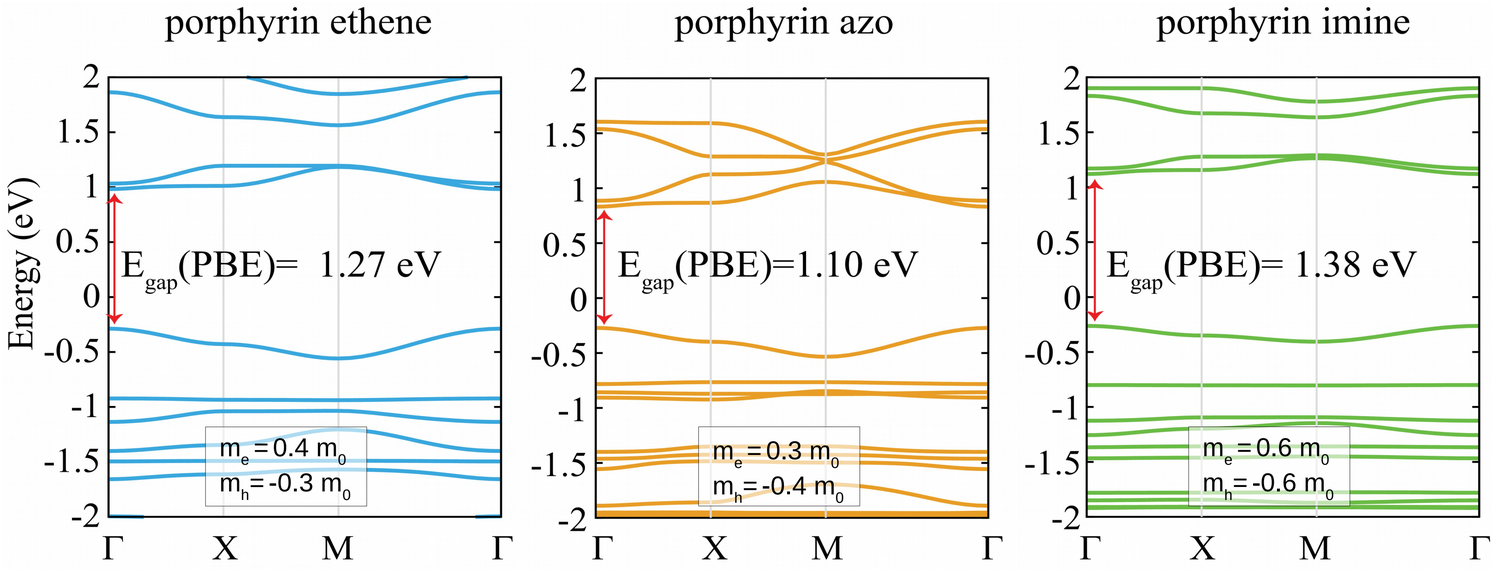
- Each COF has a quadratic unit cell. (In-plane isotropy)
- In-plane stiffness, *C*: C_{azo} = 19.8 N/m C_{imine}= 18.9 N/m C_{ethene}= 17.1 N/m

Vibrational Properties



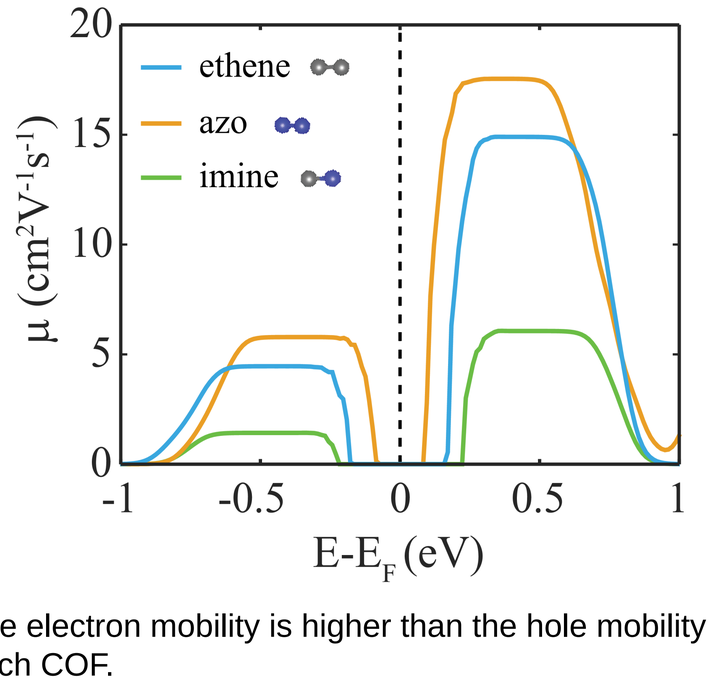
- Phonon contributions at room temperature are similar for each COF.

Electronic Properties



- Elelctronic band structures are calculated via DFT within the GGA PBE approximation.
- Each COF is a direct band gap semiconductor. Porphyrin azo has the lowest band gap.
- Porphyrin imine has larger effective mass values for both electrons and holes.

Room Temperature Mobility



- The electron mobility is higher than the hole mobility for each COF.
- Porphyrin azo has the highest mobilities, 5.8 and 17.5 $cm^2V^{-1}s^{-1}$ for holes and electrons, respectively.

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ULTIMATE ITN NETWORK

DRESDEN concept

REFERENCES

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