Elif Ünsal
Chair of Materials Science and Nanotechnology, TU Dresden

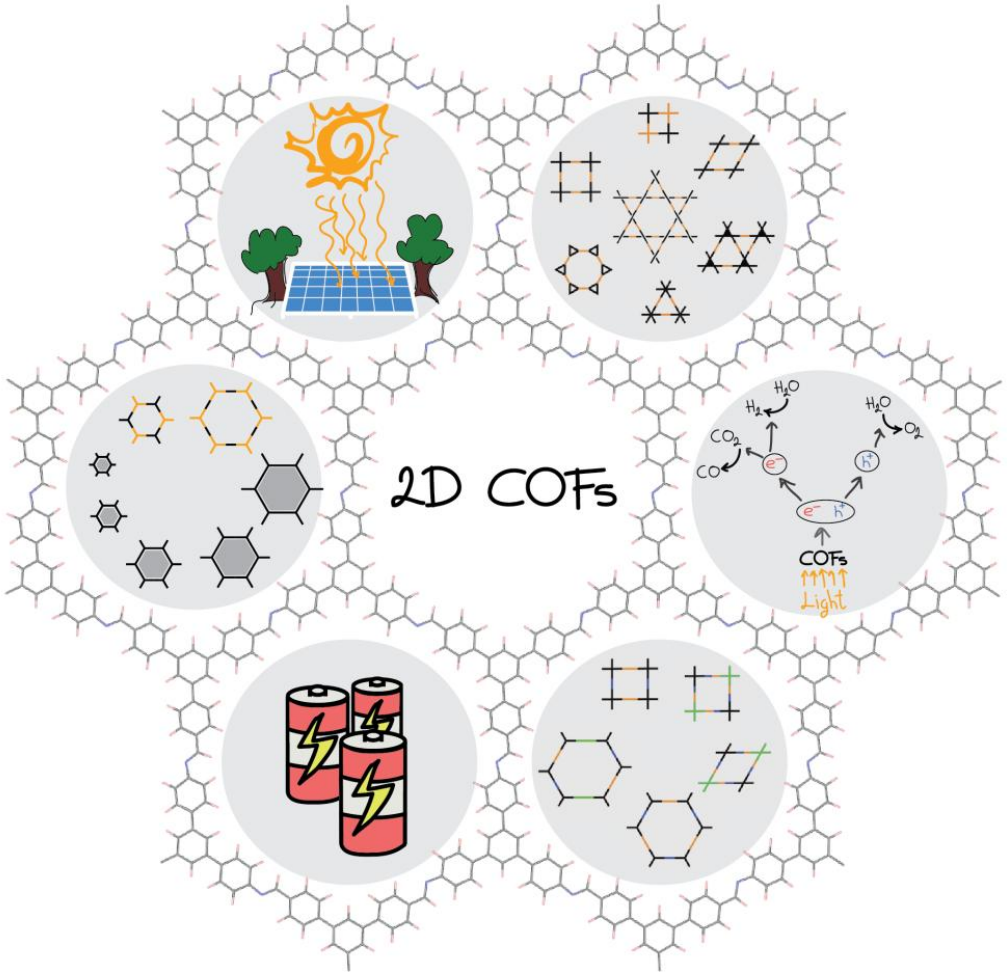
Charge Transport Mechanisms in 2D COFs

3rd TAC Meeting

Dresden, March 12th, 2024

Motivation

- 2D COFs **attractive** for **wide range** of applications in:
  Photovoltaics, energy storage, catalysis etc.



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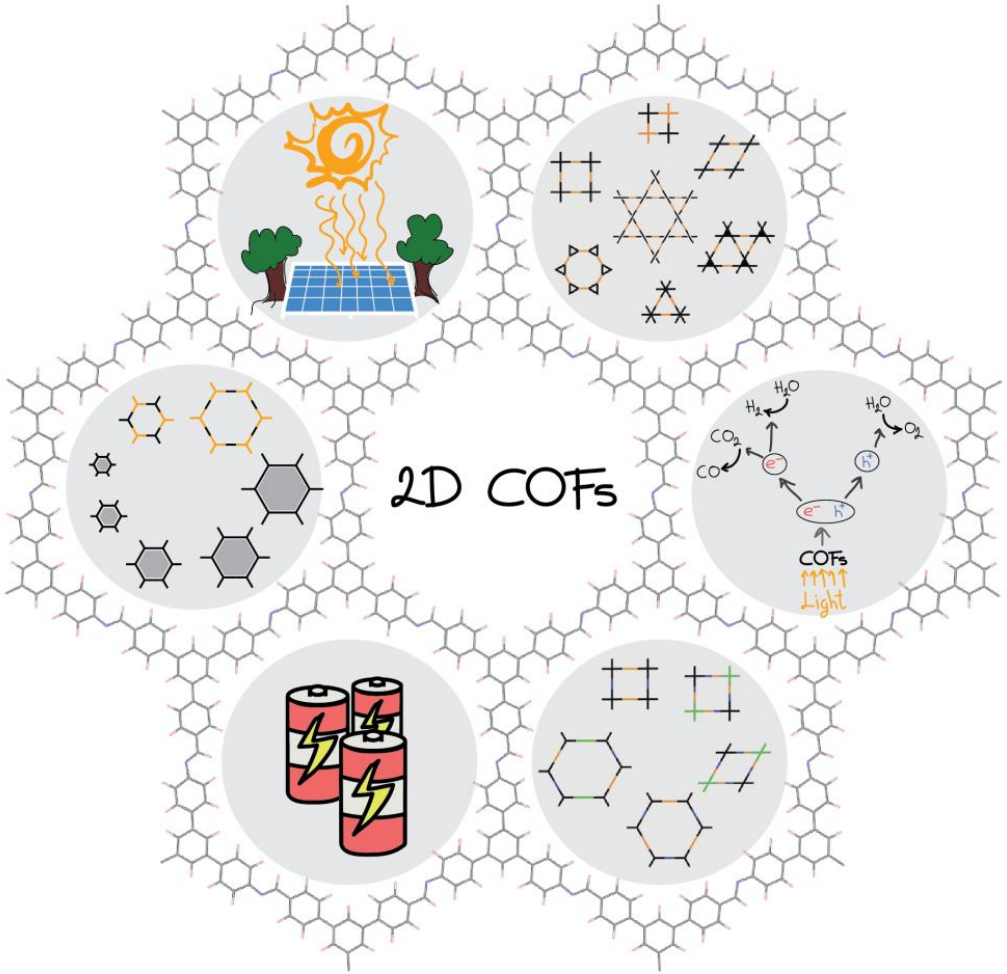
- **Various types** of tailor-made 2D COFs



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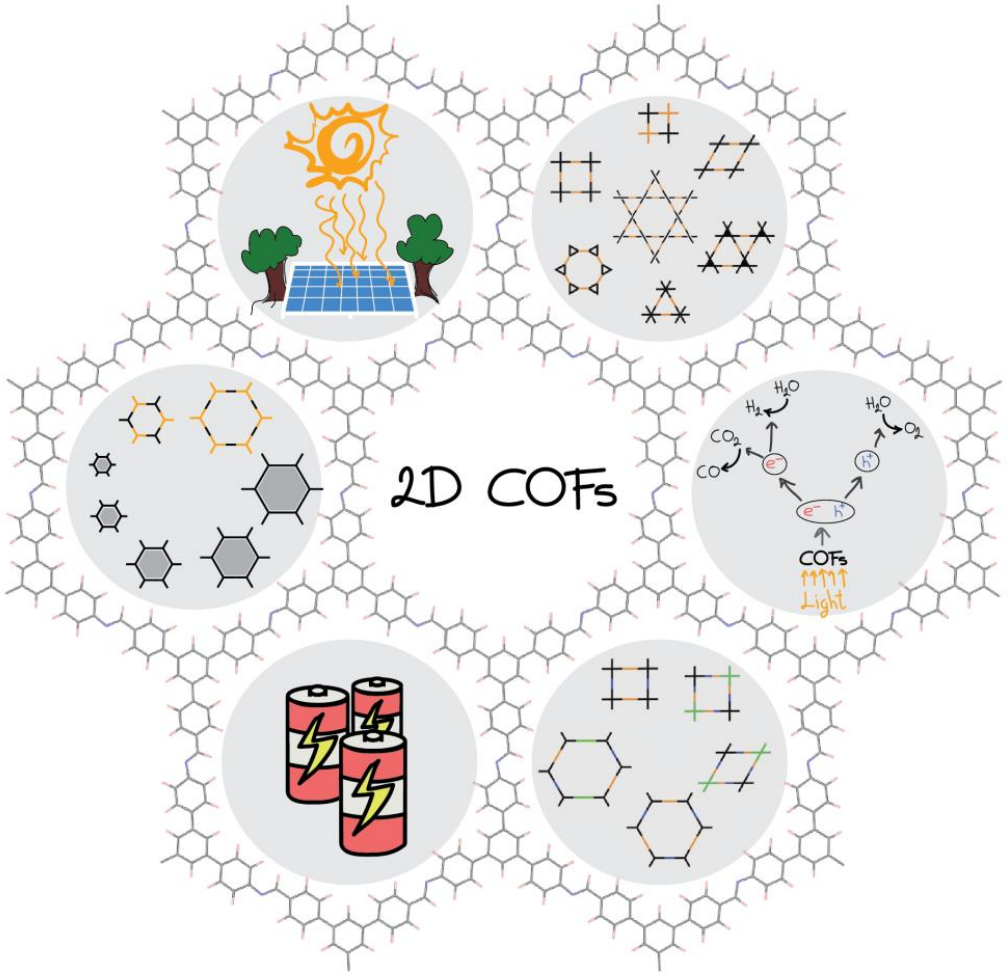
- **Feasibly tunable** physical properties!



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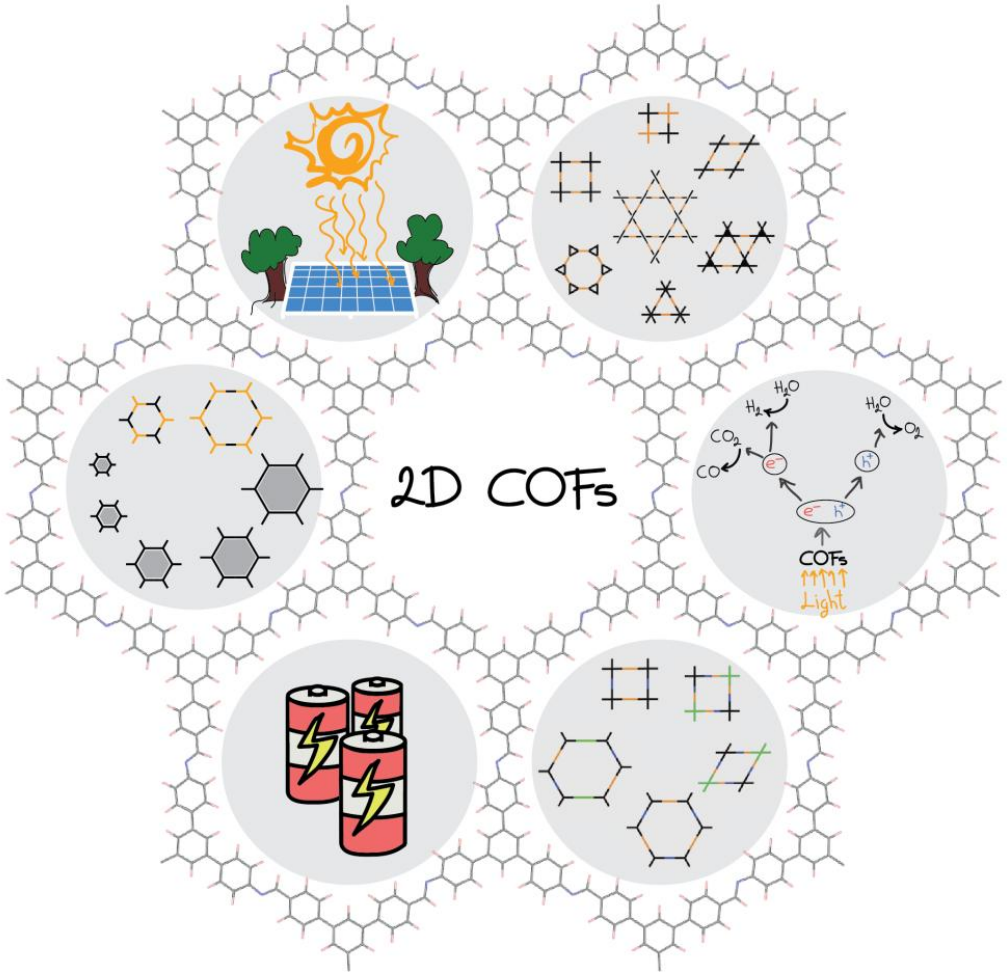
- **Huge** variety of COFs **!!**
  Systematic investigation
  Predicting the promising materials



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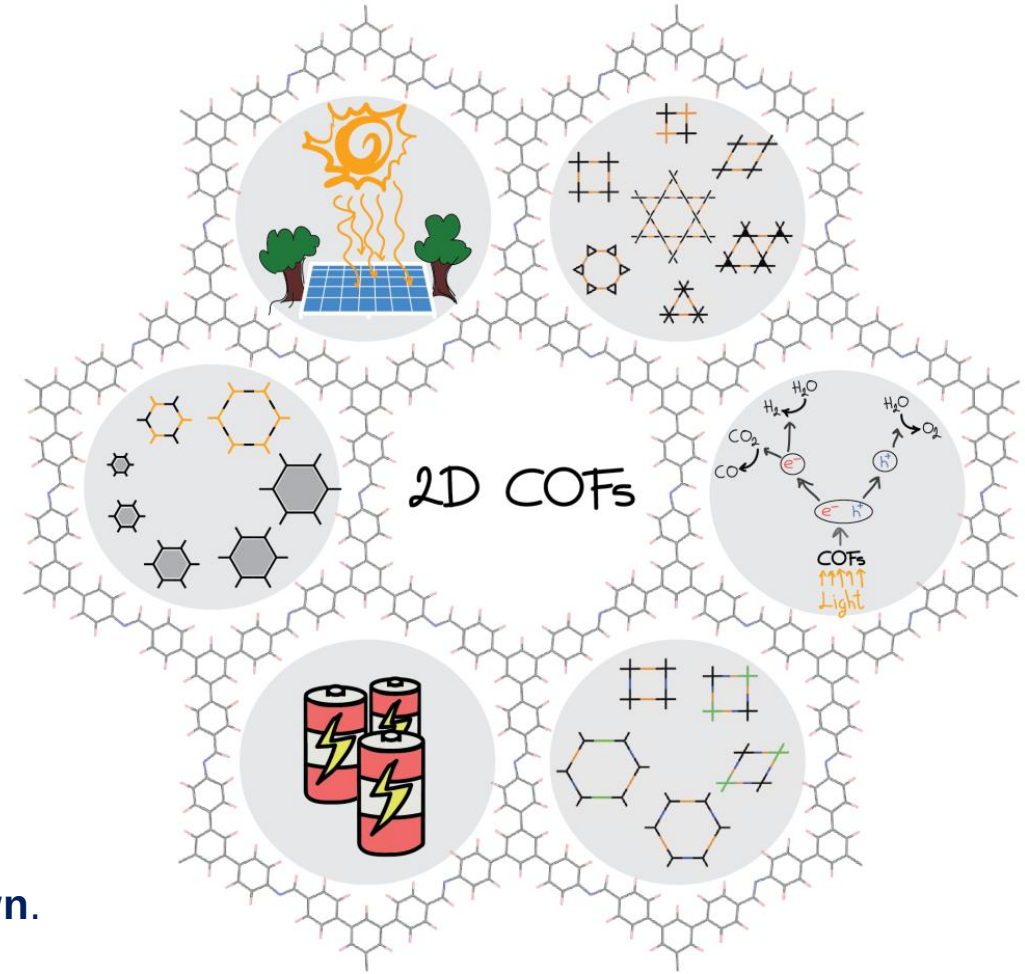
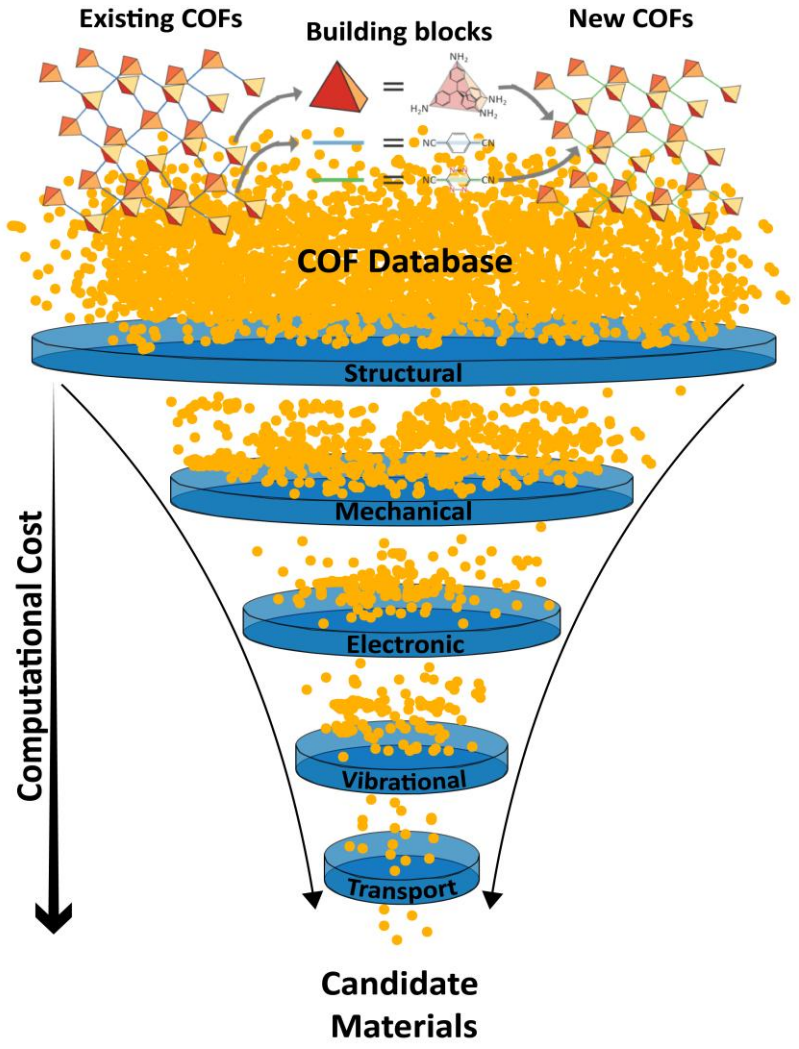
  Systematic investigation
  Predicting the promising materials
- **Charge transport** properties of most of 2D COFs are **still unknown**.



Objectives & Challenges

- To **understand** **the charge transport** mechanisms in 2D COFs using **first-principle approaches**



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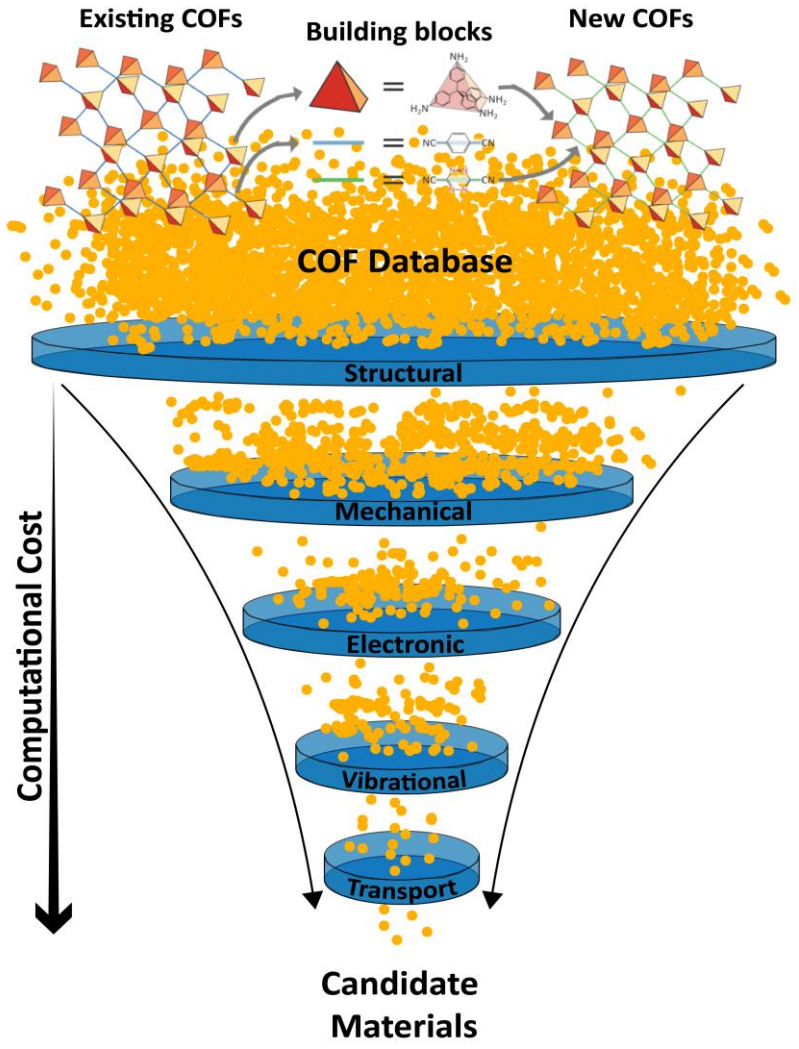
- To **understand** **the charge transport** mechanisms in 2D COFs using **first-principle approaches**

- To **design** novel 2D COFs with **functional transport properties**



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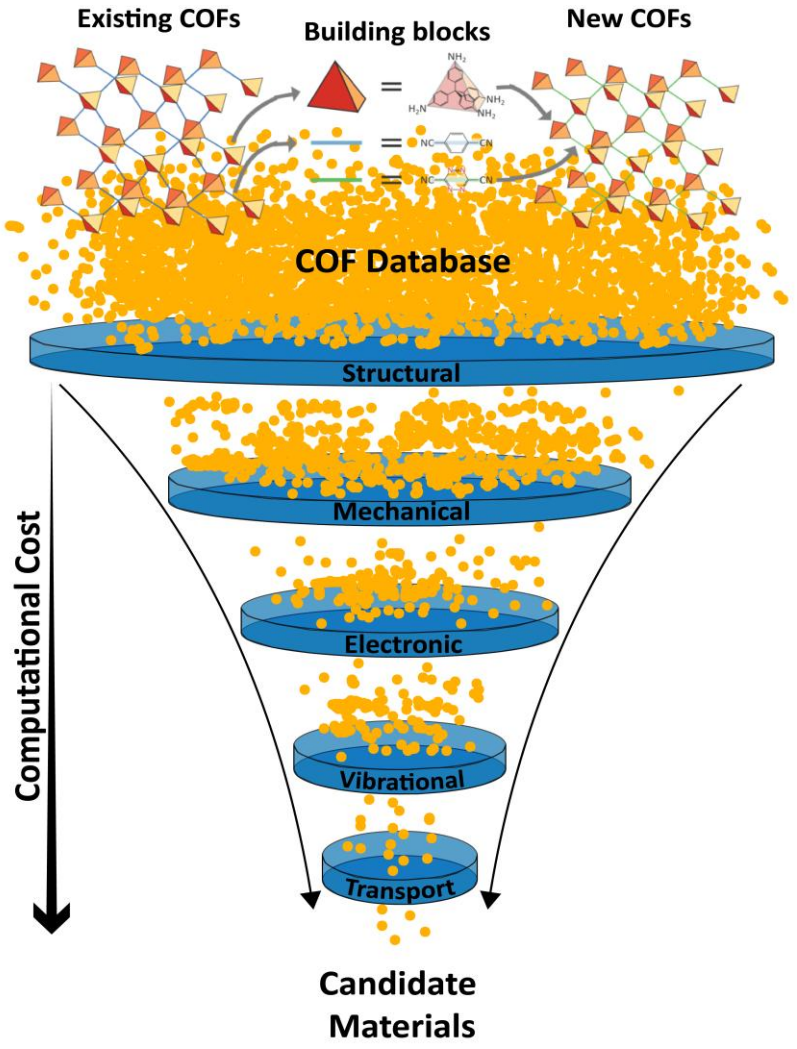

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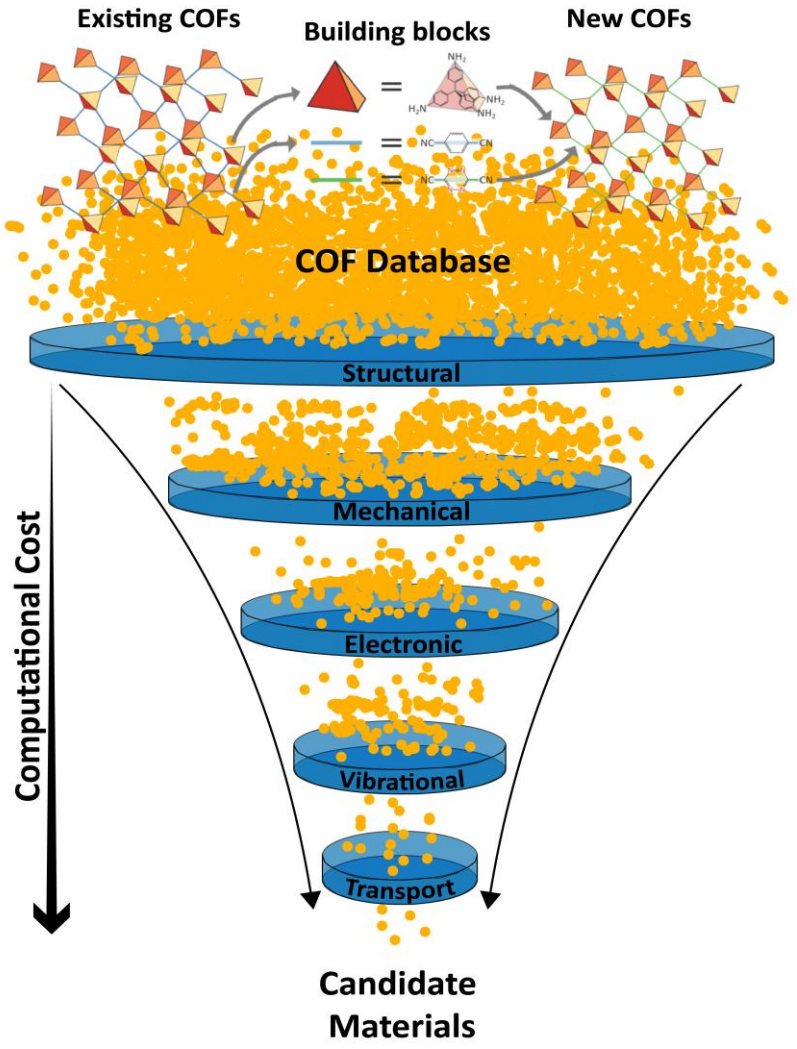

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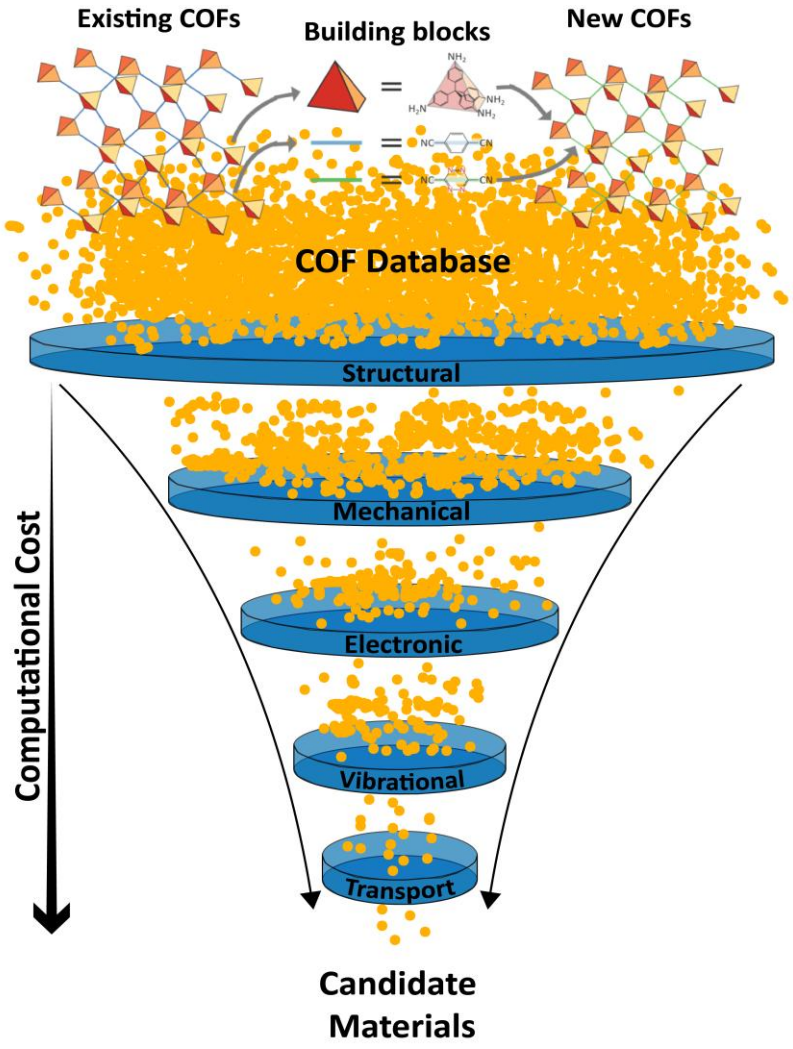
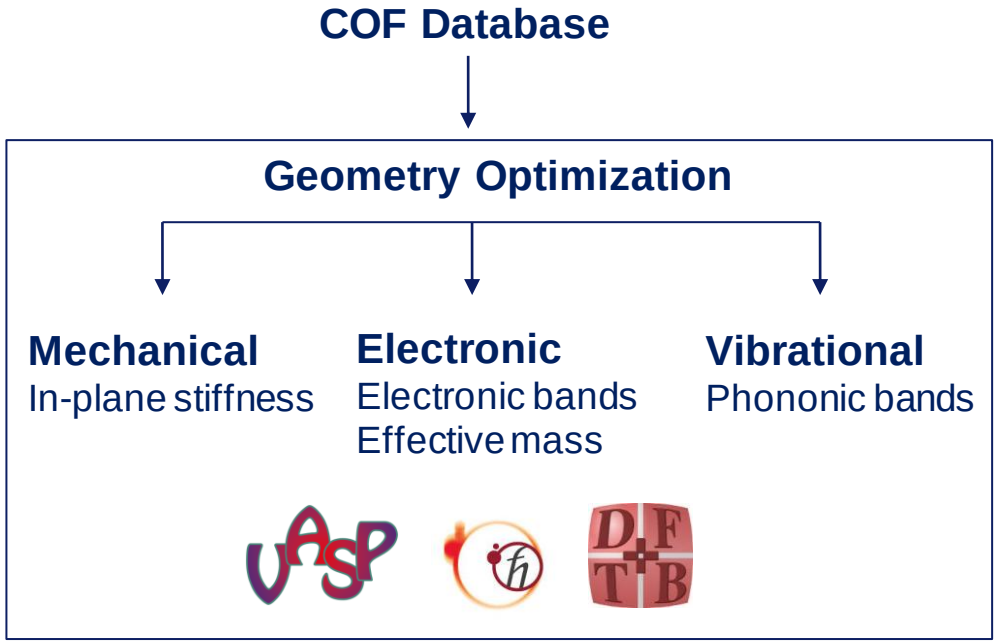
Semi-empirical methods
(such as DFTB) → **much faster**
than DFT approaches



Methodology



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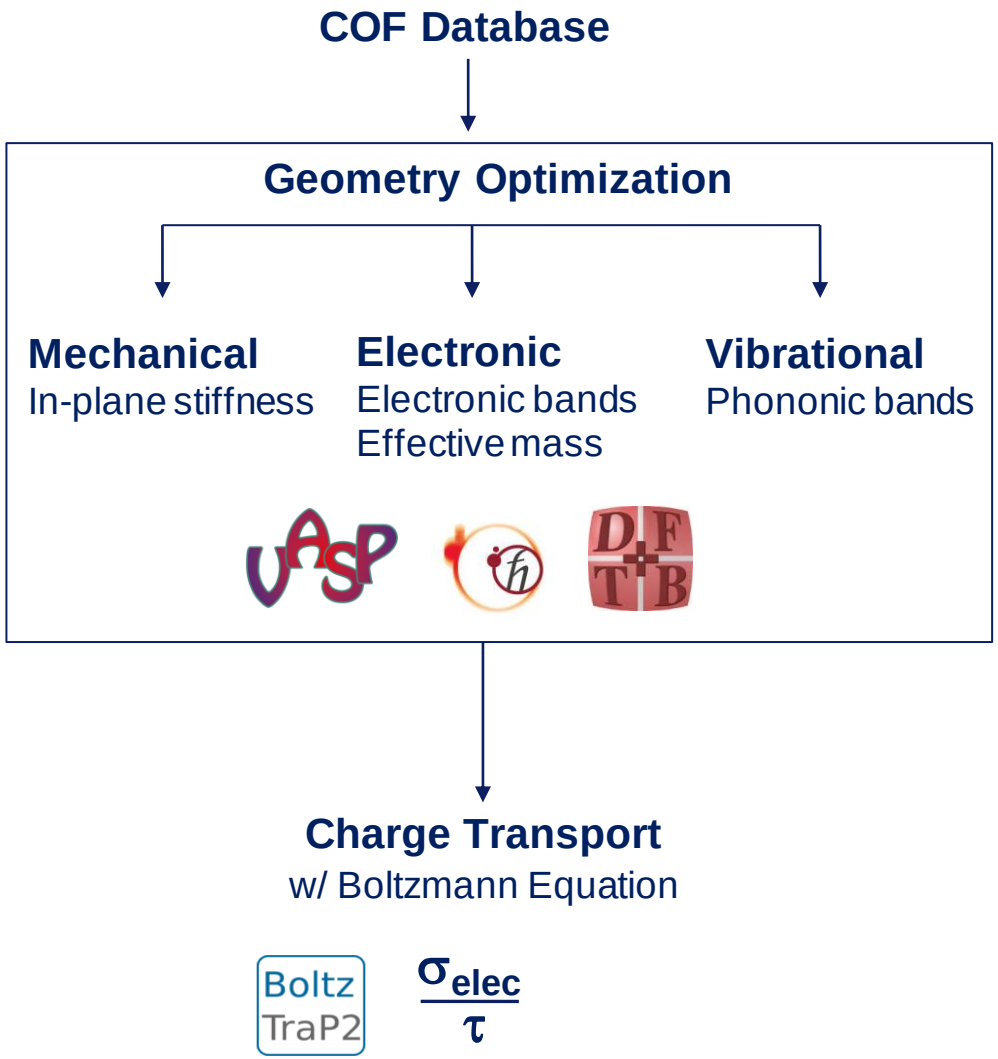

Methodology

COF Database

Geometry Optimization

Mechanical
In-plane stiffness

Electronic
Electronic bands
Effective mass

Vibrational
Phononic bands

Charge Transport
w/ Boltzmann Equation

BoltzTraP2

σ_{elec} / τ

Relaxation Time Approximation (RTA)

Constant RTA
Acoustical Deformation Potential Theory

$$\tau_{2D} = \frac{\hbar^3}{k_B T}\left(\frac{C_{2D}}{m^* D^2}\right)$$

Self-energy RTA
Electron-Phonon Coupling (**EPC**) Calculations

EPW

dftbephy

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Geometry Optimization

Mechanical
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$\frac{\sigma_{elec}}{\tau}$

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Self-energy RTA
Electron-Phonon Coupling (**EPC**) Calculations

EPW

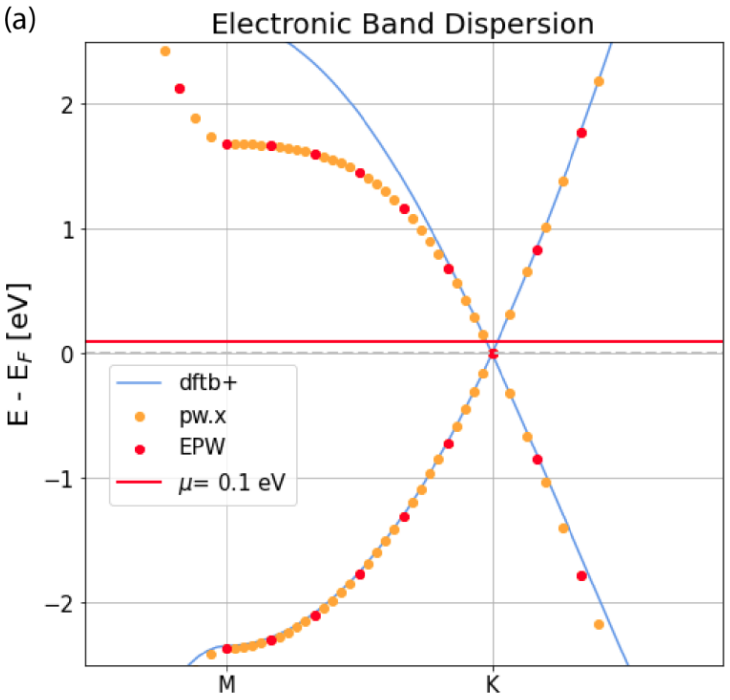
dftb ephy

Estimated τ

Electrical conductivity
Mobility

Results

Benchmarking Scattering Rates in Graphene: DFTBephy vs EPW



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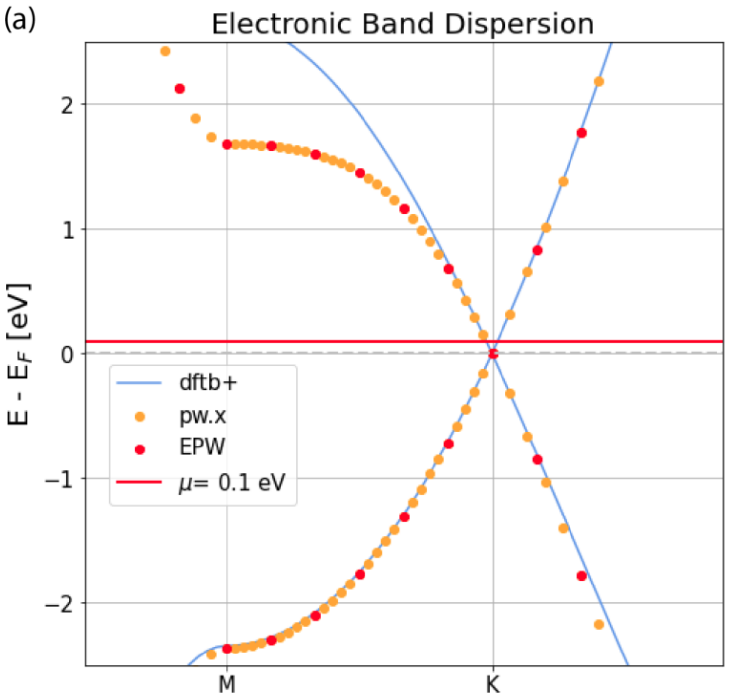

Values between -0.4 and 0.4 eV in a **good agreement**

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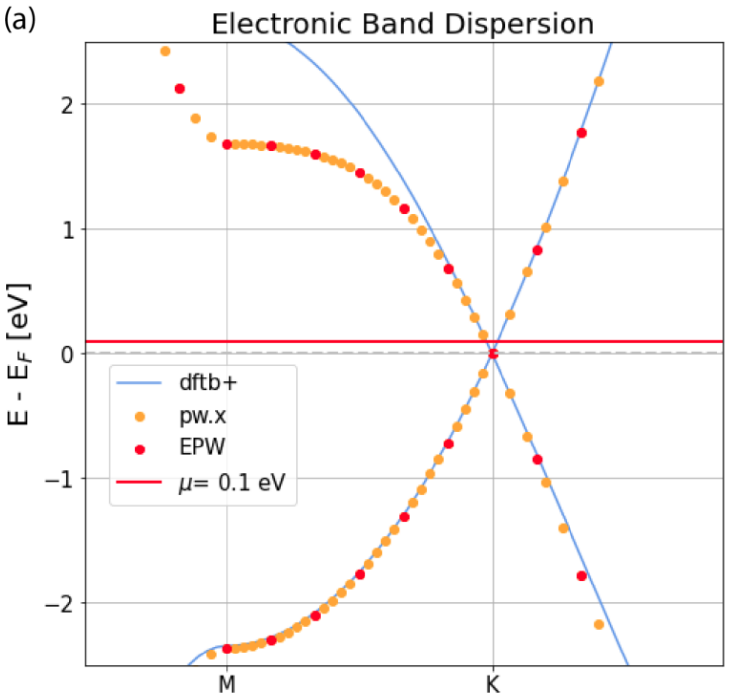

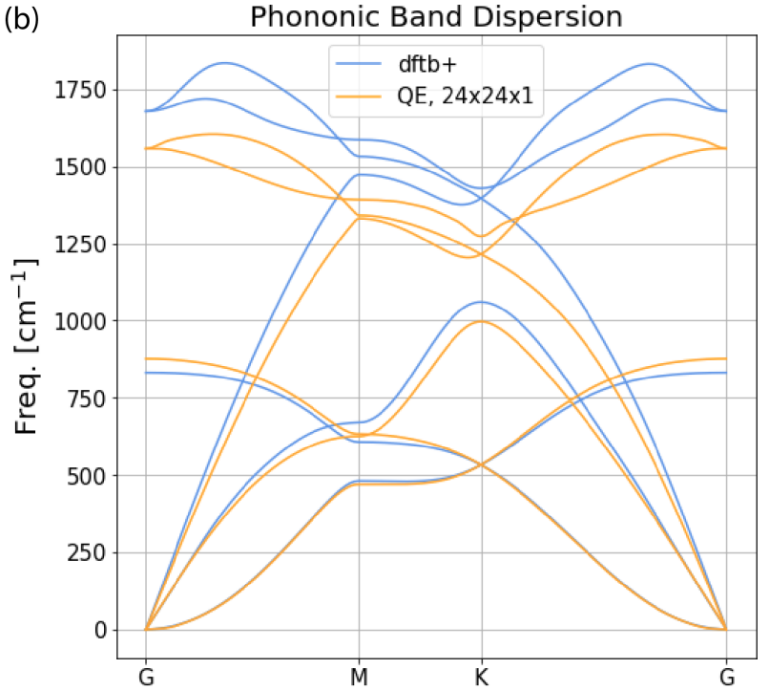

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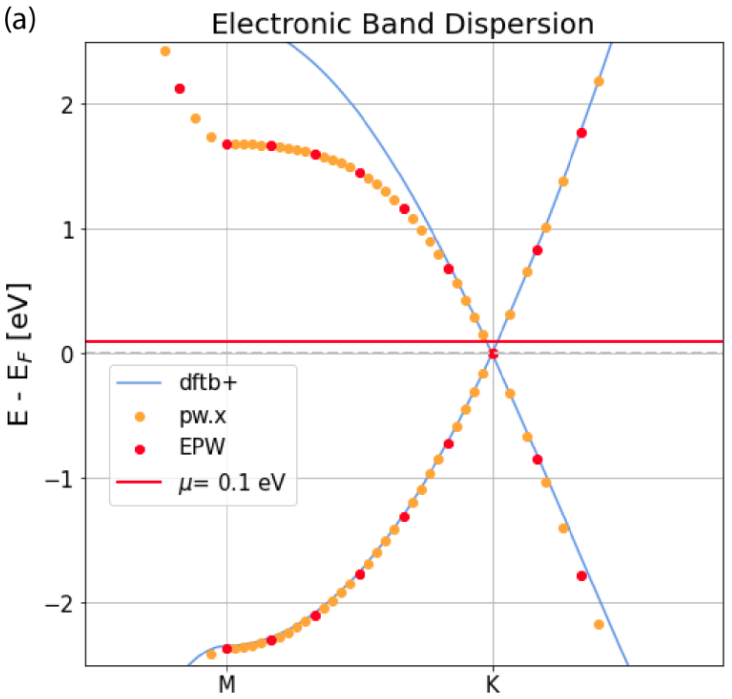

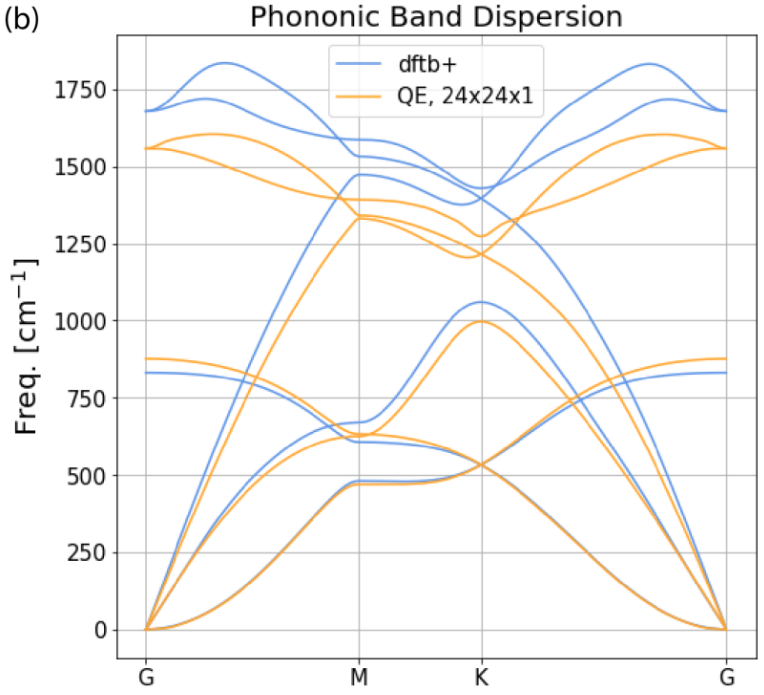

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Compatible acoustic phonon dispersion around Γ

- Lower **ZO**
- Higher **LO** and **TO**

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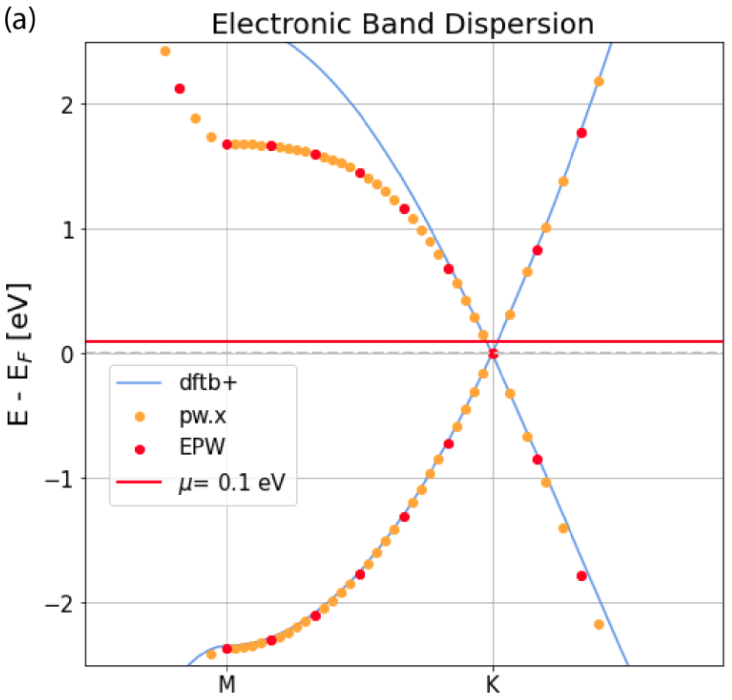

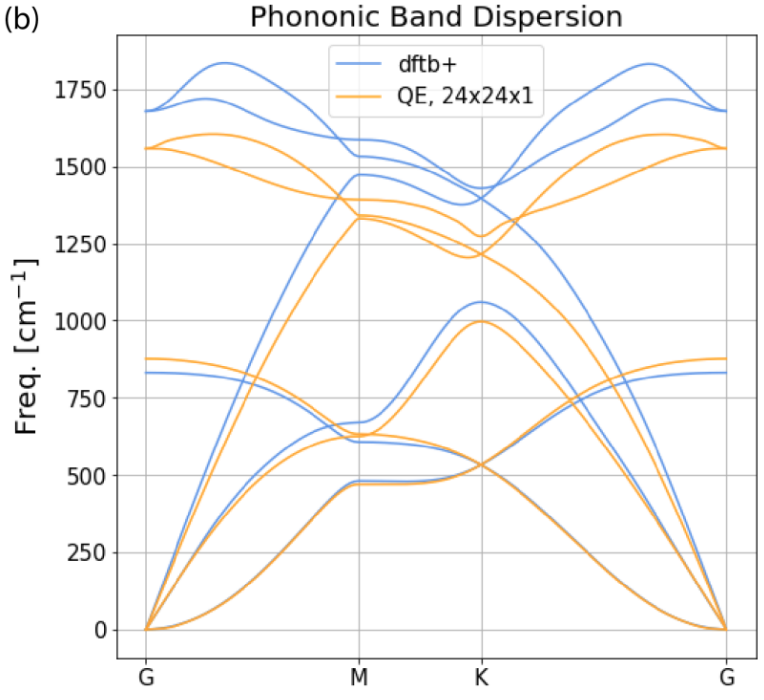

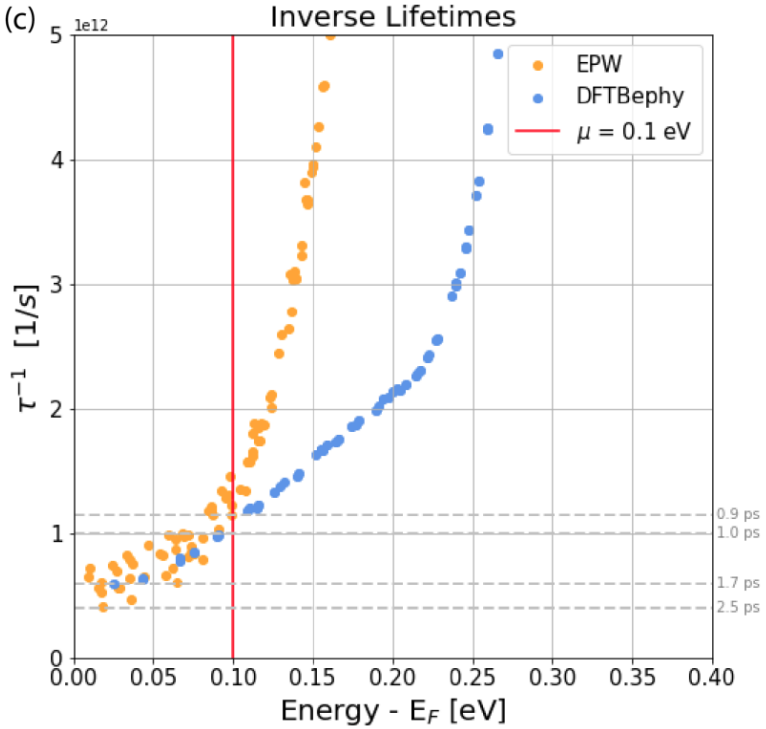

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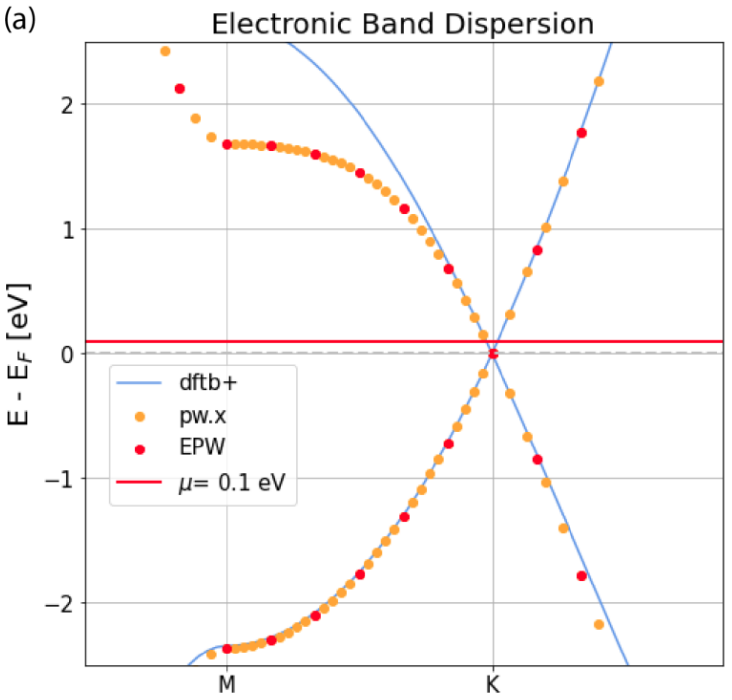

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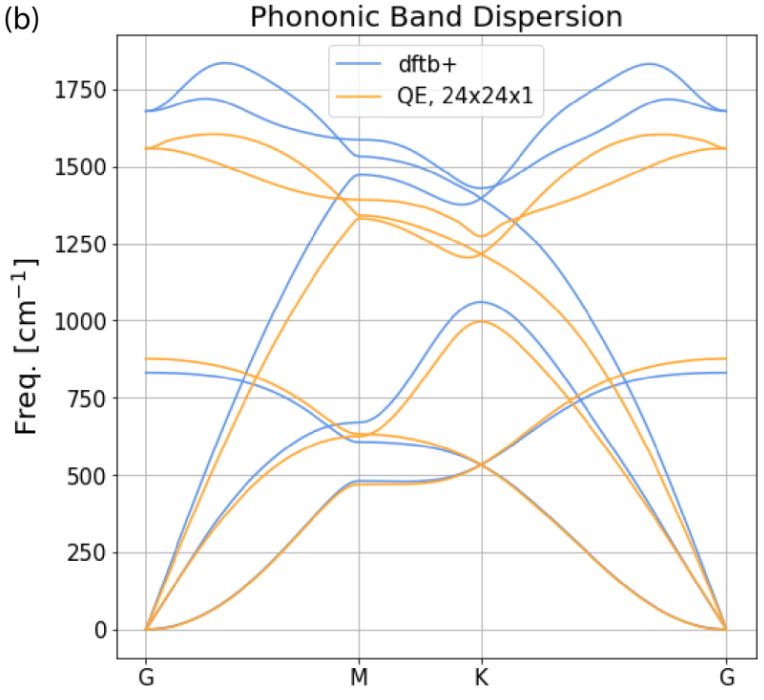

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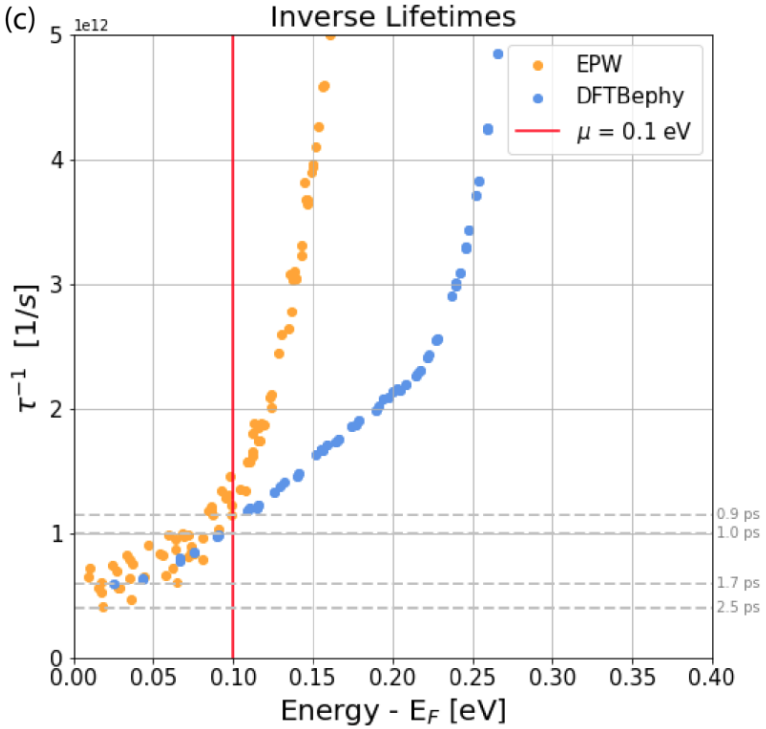

τ in the same order of magnitude!

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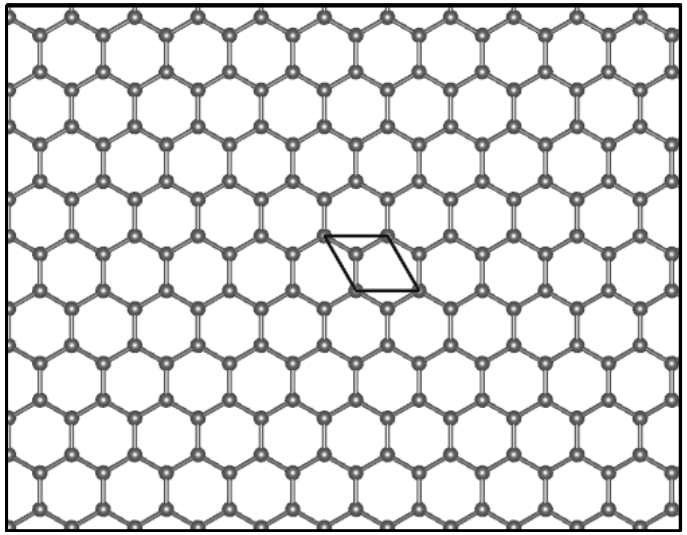
Graphene and 2D Graphene Allotropes

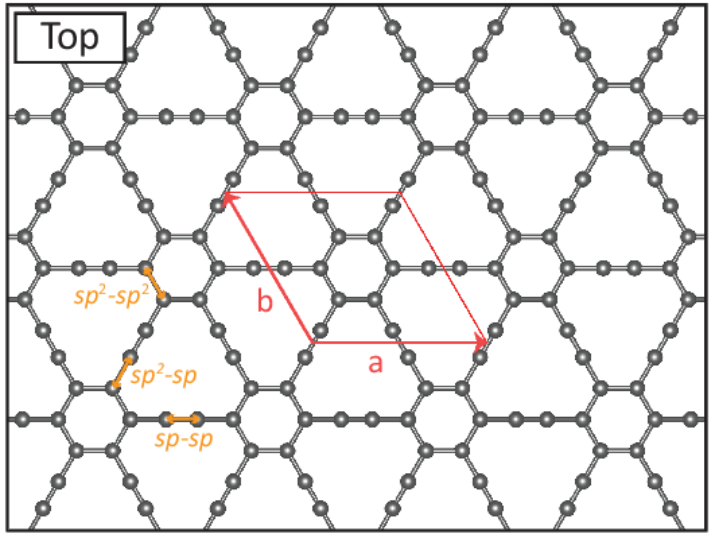
(a) Graphene



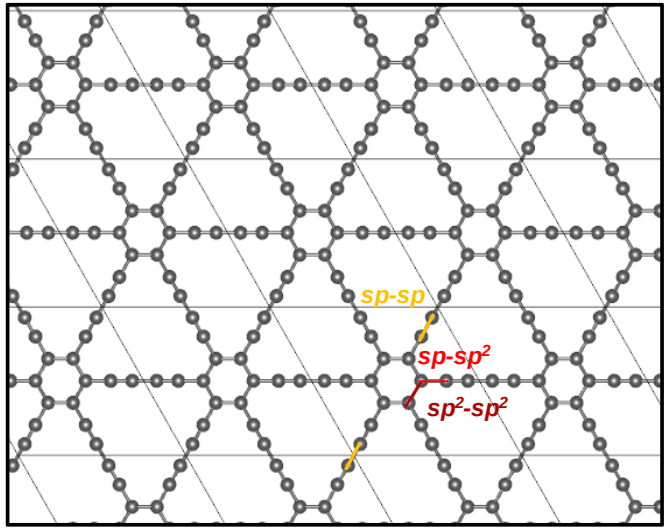
a= 2.42 Å uc: 2 atoms

Semi-metal
Dirac point at *K*

(b) γ-Graphyne



(c) Graphdiyne (GDY)



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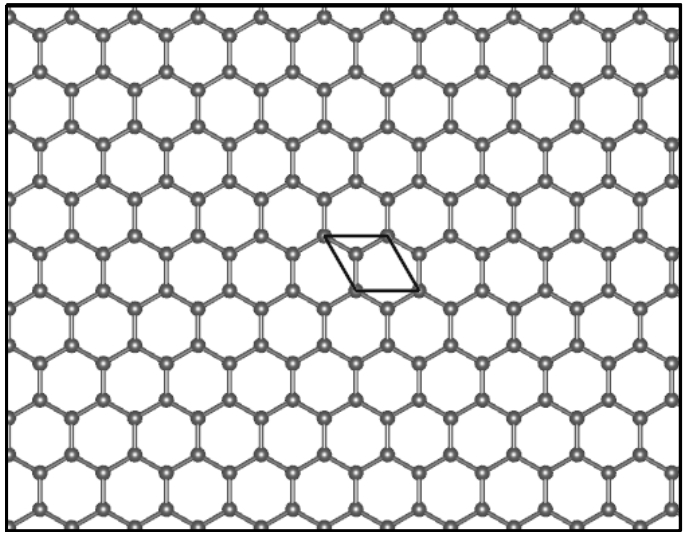

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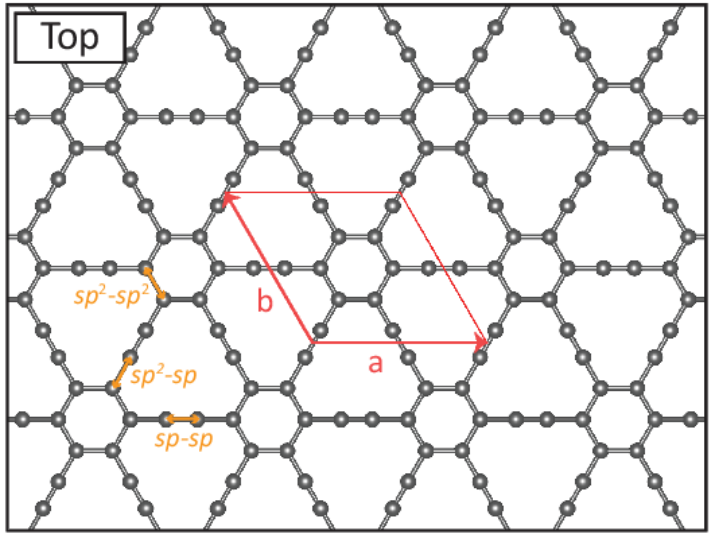

a= 6.92 Å uc: 12 atoms

Direct band gap at *M*
E_{gap} (PBE) = 0.46 eV
E_{gap} (mio) = 1.38 eV

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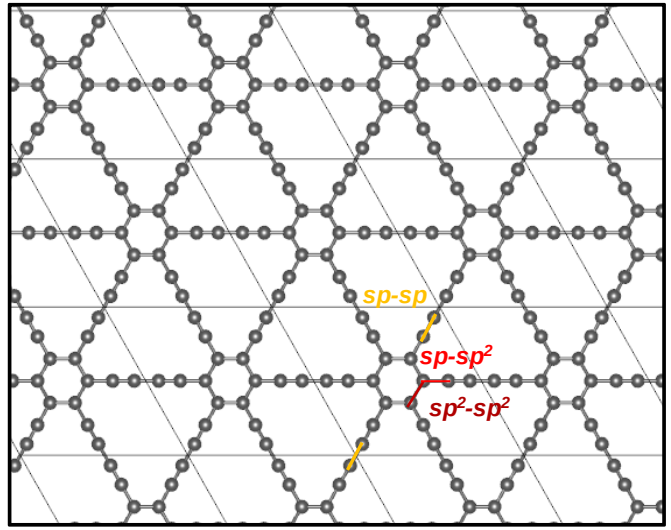

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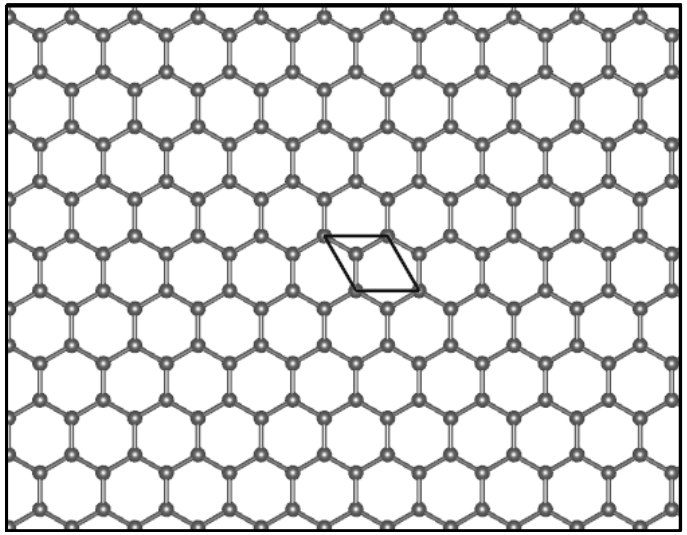

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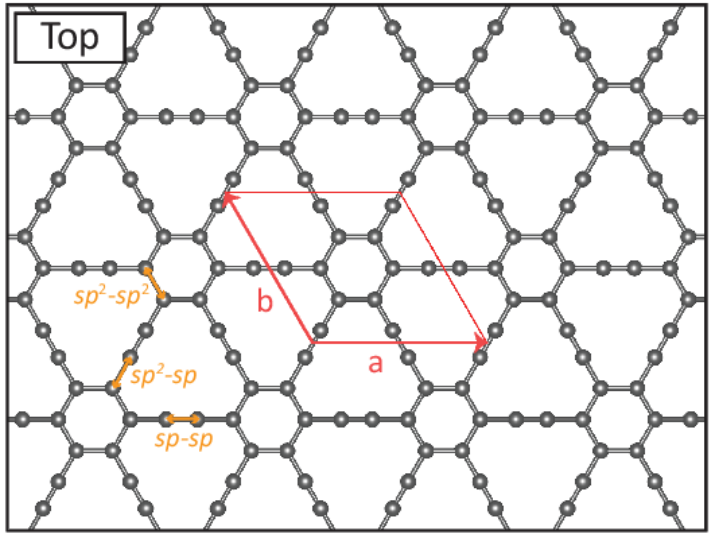

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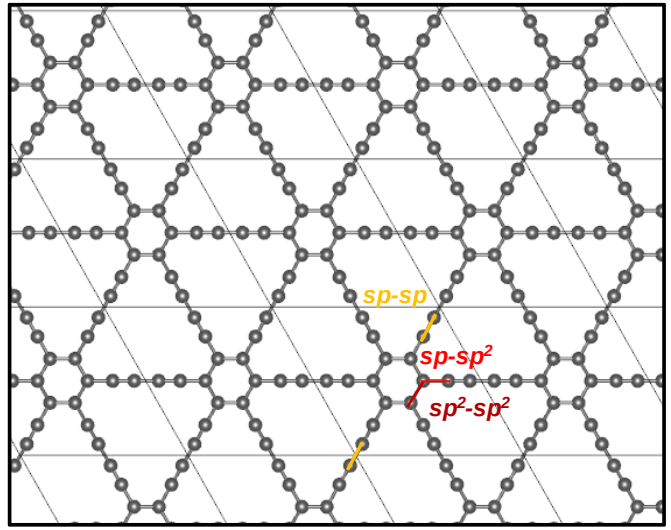

a = 9.53 Å uc: 18 atoms

Direct band gap at Γ
E_{gap} (PBE) = 0.48 eV
E_{gap} (mio) = 1.52 eV

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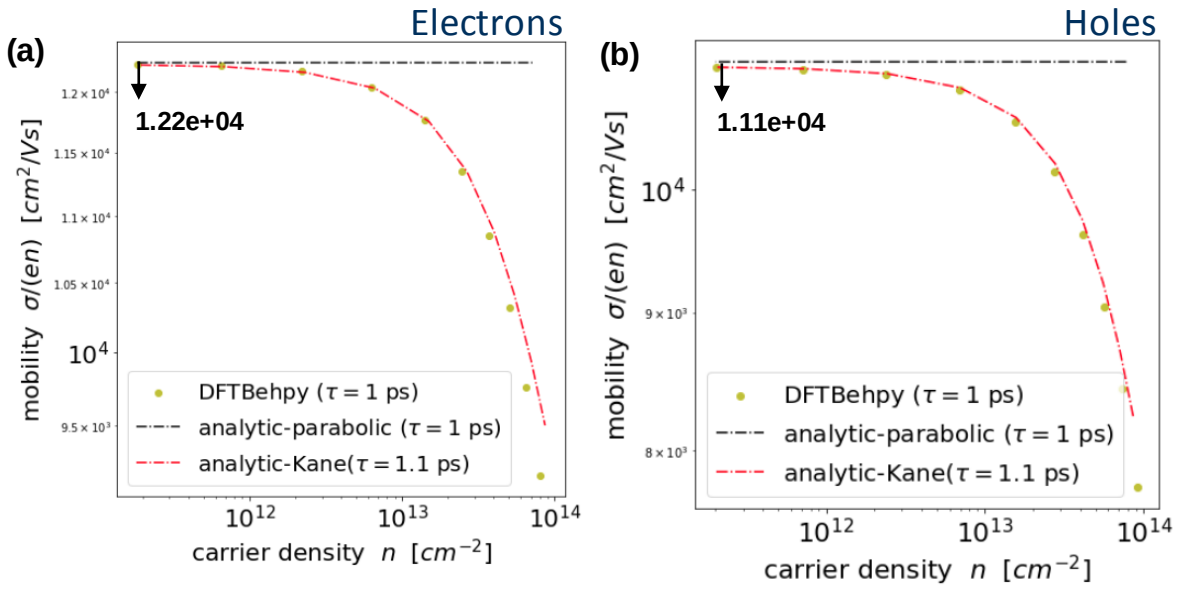
2D Graphene Allotropes: Room Temperature Mobilities w/ CRTA

γ-Graphyne



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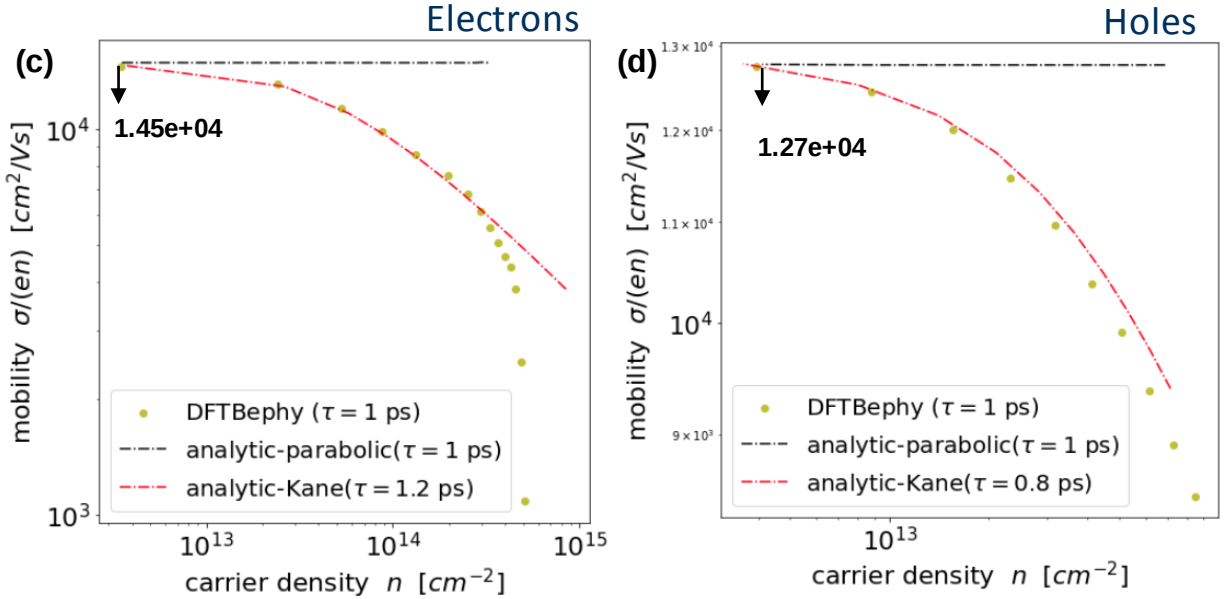

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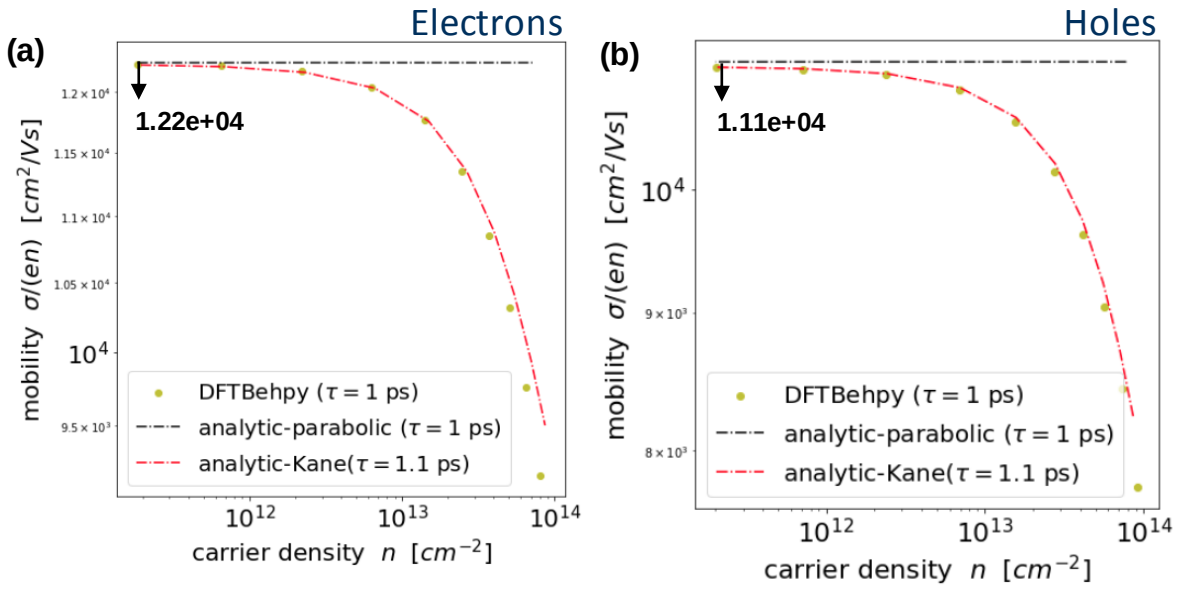

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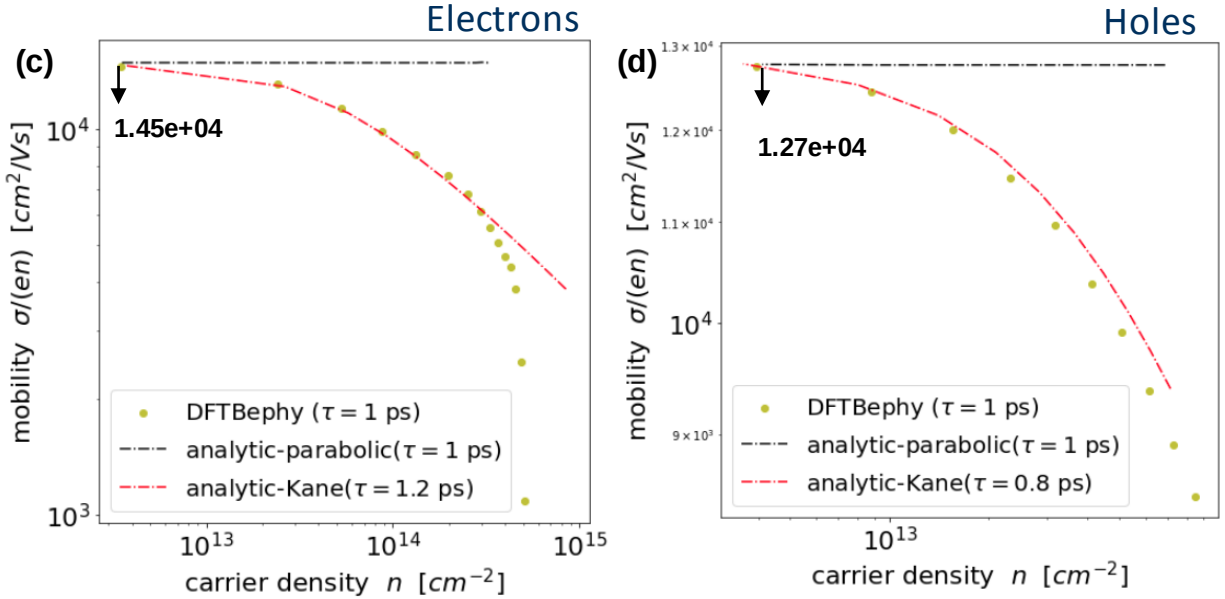

In both materials:

μ(elec) > μ(holes) ⟶ but not an order of magnitude!

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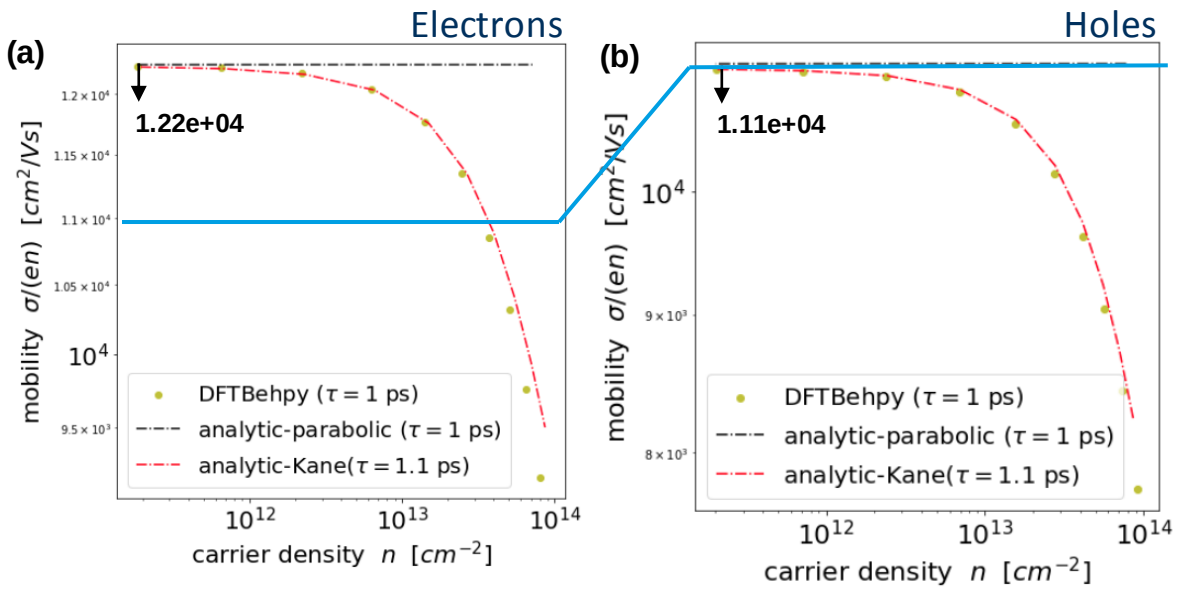

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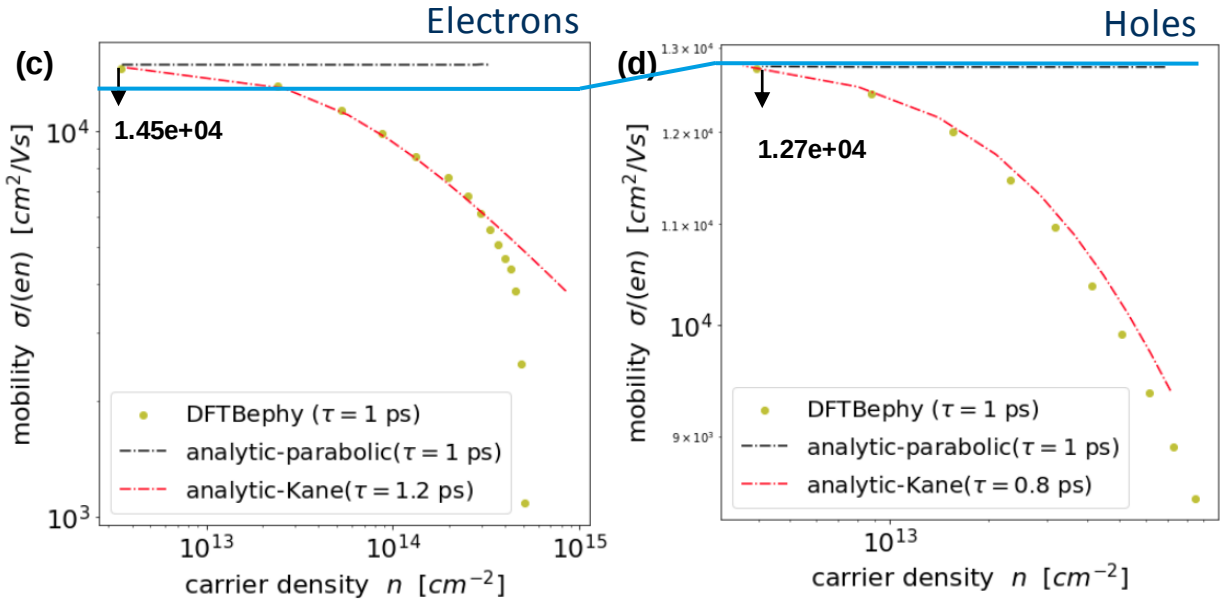

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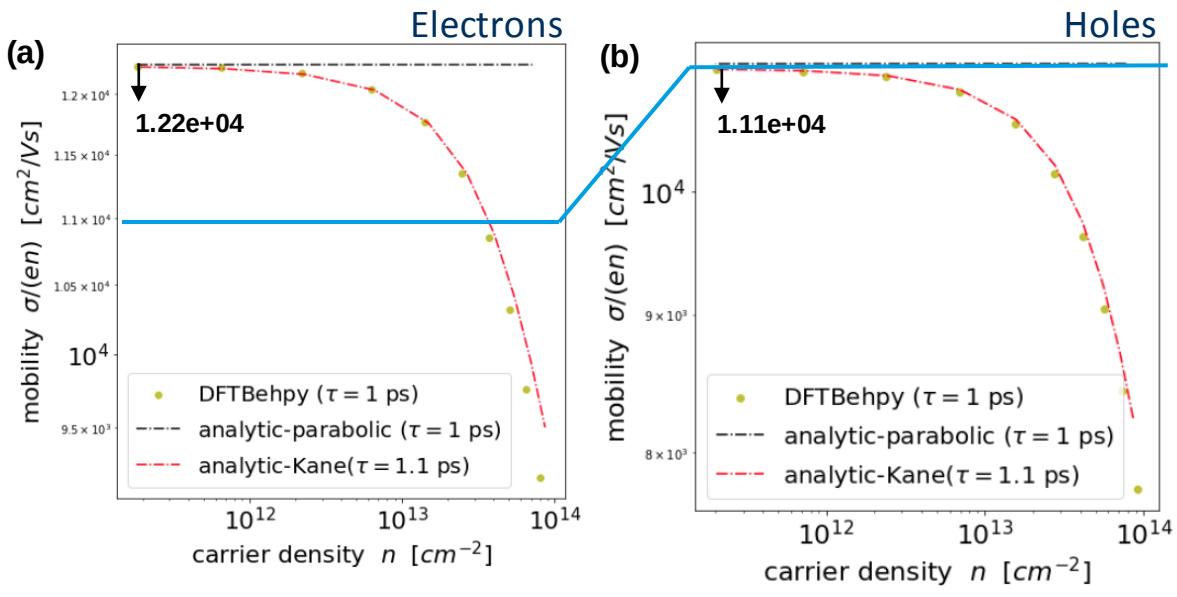

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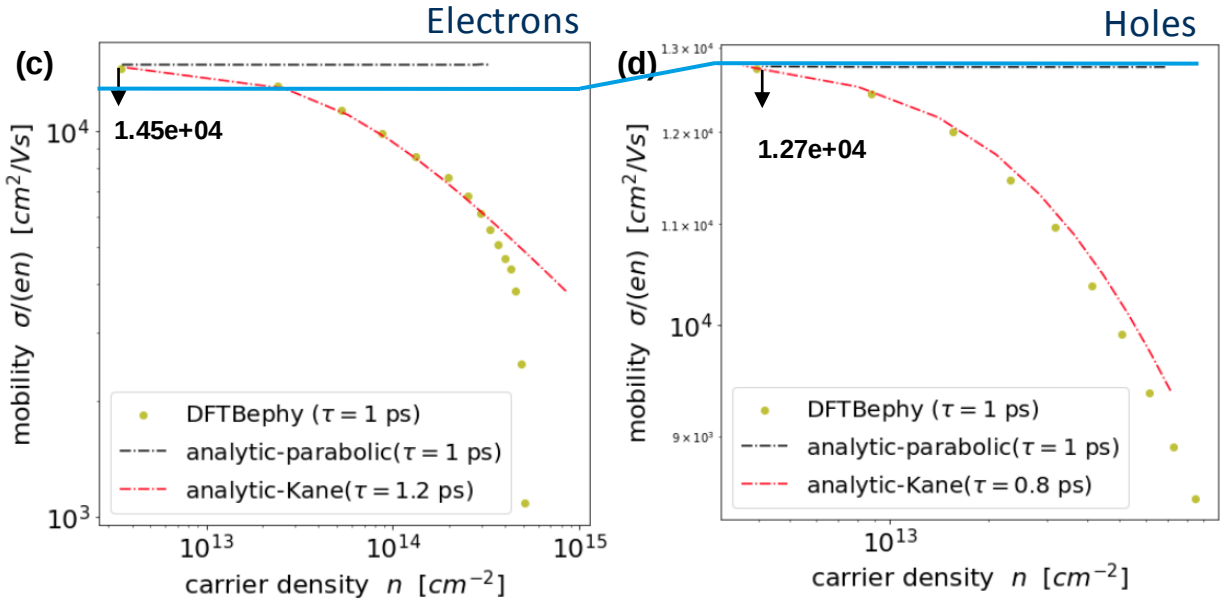

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Predicted: μ(elec) ≈ 10^5 cm^2/Vs, μ(hole) ≈ 10^4 cm^2/Vs
(*Boltzmann transport equation+ deformation potential*)

J. Chen, J. Xi, D. Wang, and Z. Shuai **J.Phys.Chem.Lett. 2013**, 4, 9, 1443-1448.
M. Long,L. Tang,D. Wang,Y. Li, and Z. Shuai **ACS Nano 2011**, 5, 4, 2593-2600.

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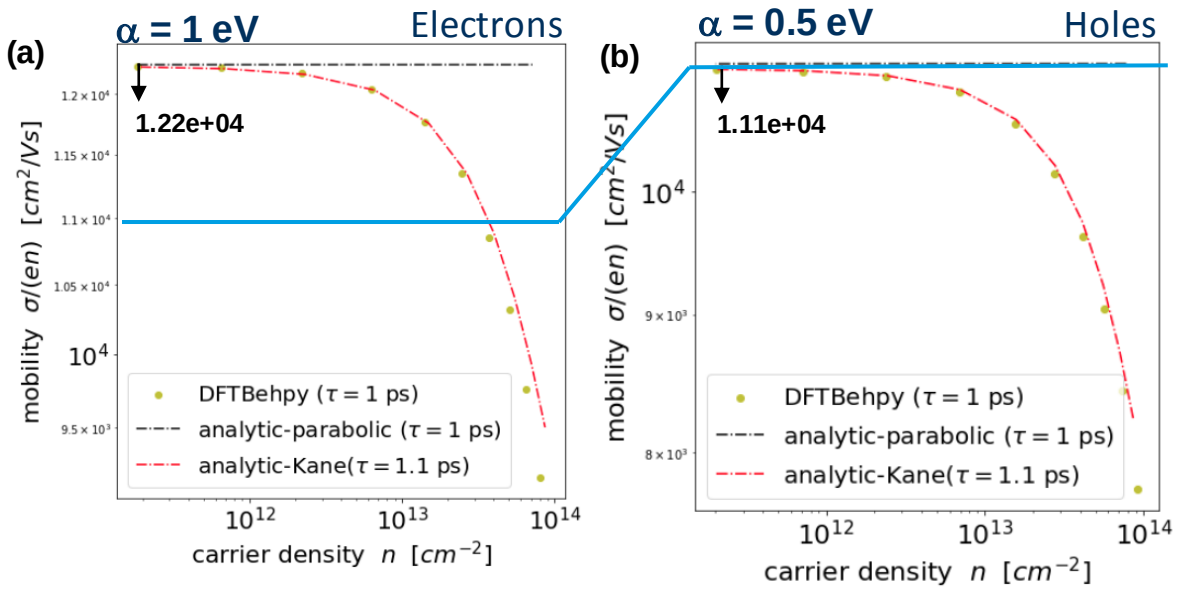

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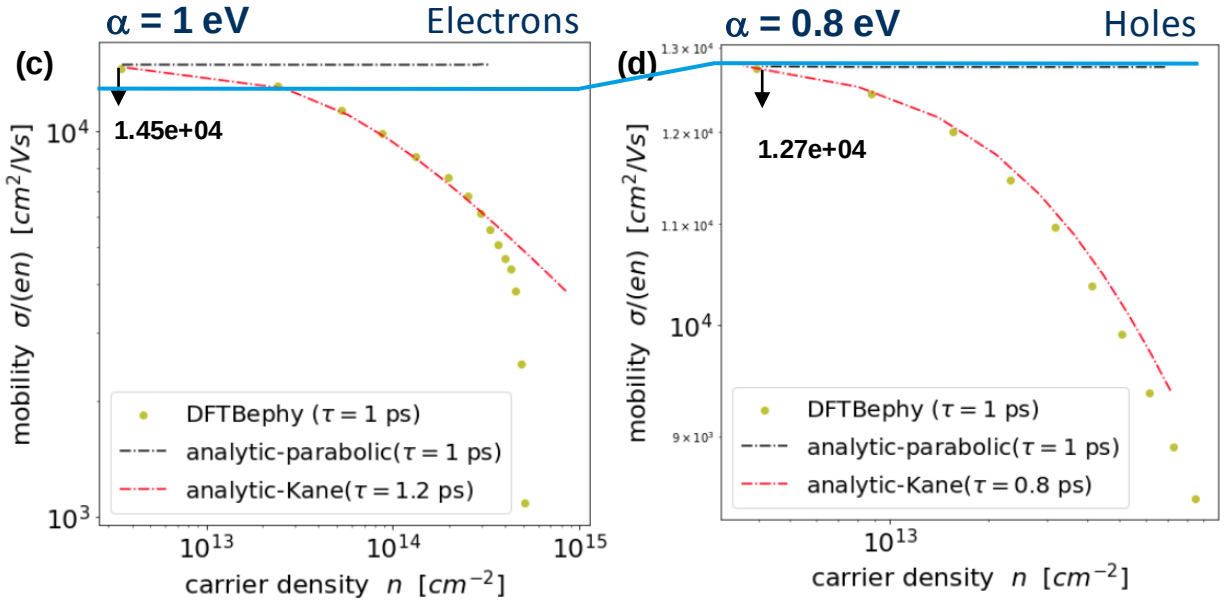

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Kane Dispersion: $\varepsilon(1+\alpha\varepsilon) = \frac{\hbar^2\mathbf{k}^2}{2m}$

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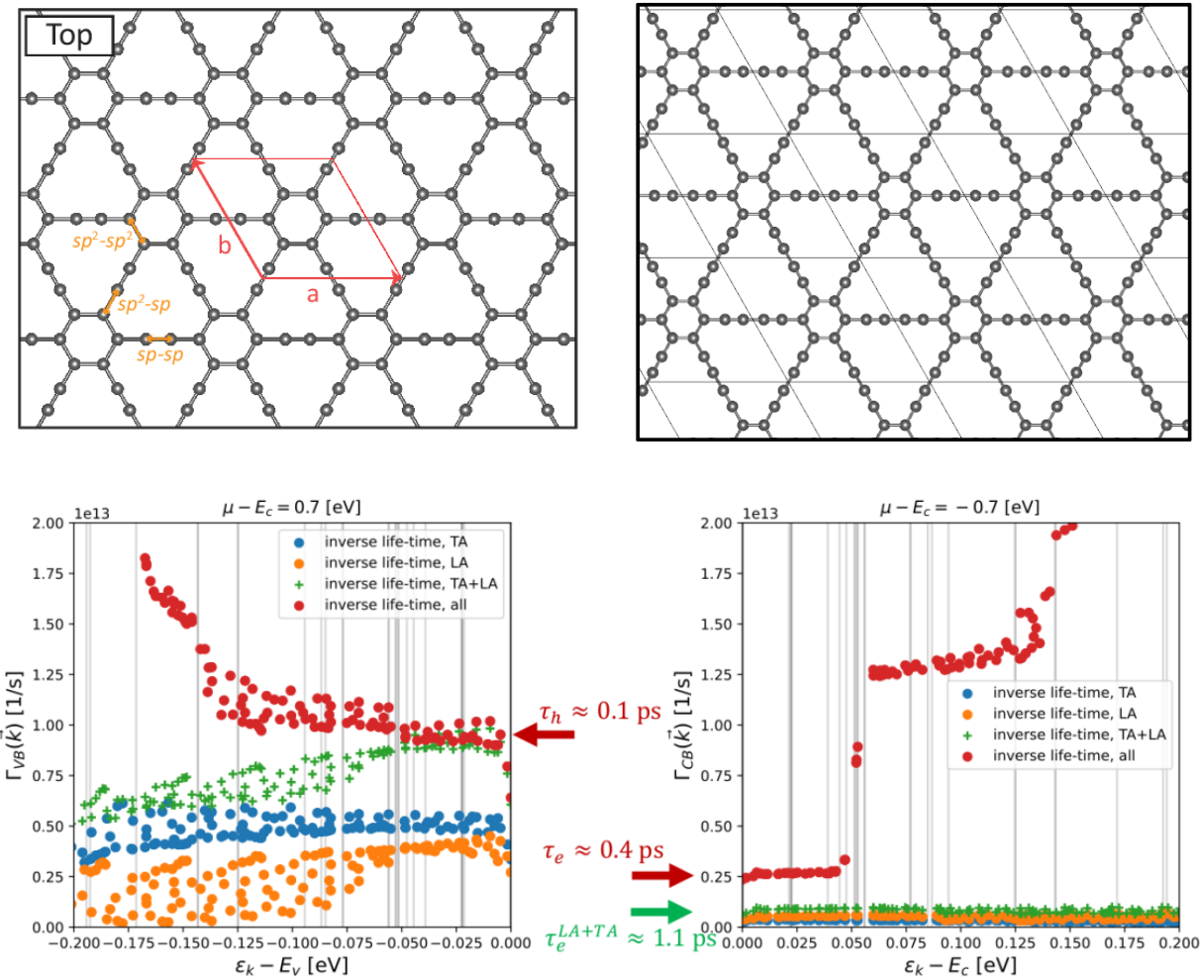
Results

2D Graphene Allotropes: Beyond CRTA



On-going work:

w/ SERTA

- Relaxation-times
- Carrier Mobilities

Temperature-dependent carrier mobilities

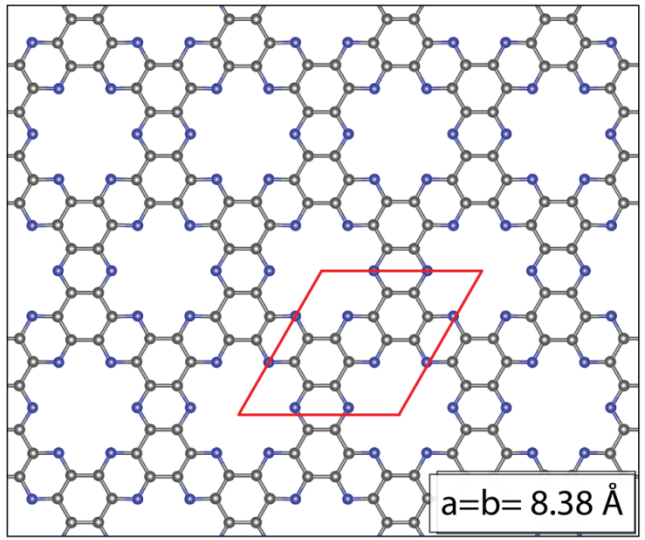
Impact of non-parabolicity on mobility

Results

2D Hexagonal C_2N COF

Optimized Geometry

(a)



18 atoms in the unit cell

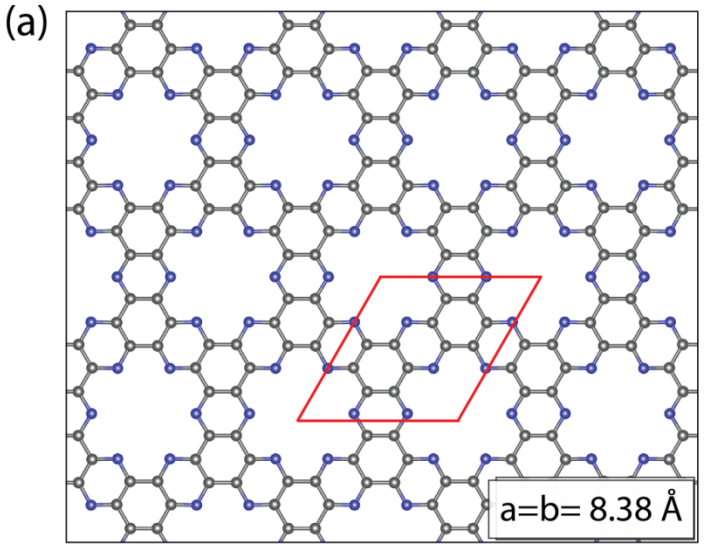
- Synthesized with high crystallinity
- Relatively high carrier moblities
- Promissing material for device applications

J. Mahmood, Jong-Beom Baek,Nat. Commun. 6, 6486, 2015.

Results

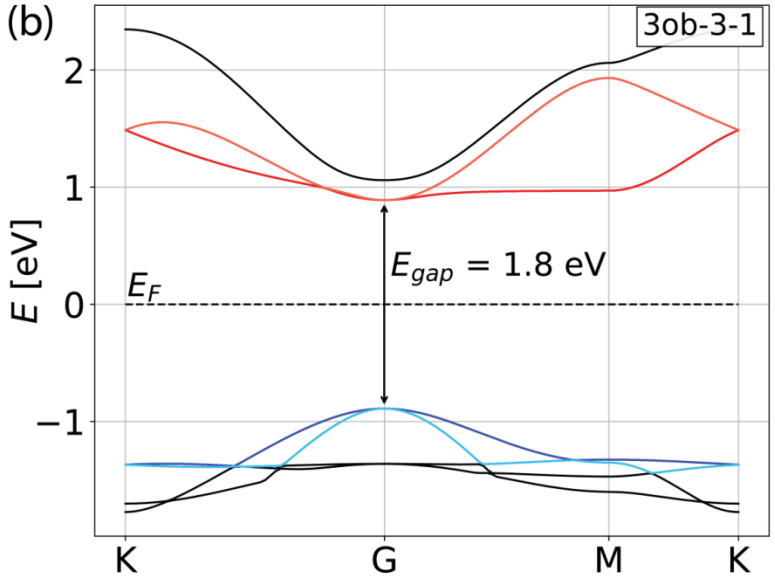
2D Hexagonal C_2N COF

Optimized Geometry



18 atoms in the unit cell

Electronic Properties



Degeneracy at the band edges
Egap (Expt.) = 1.96 eV

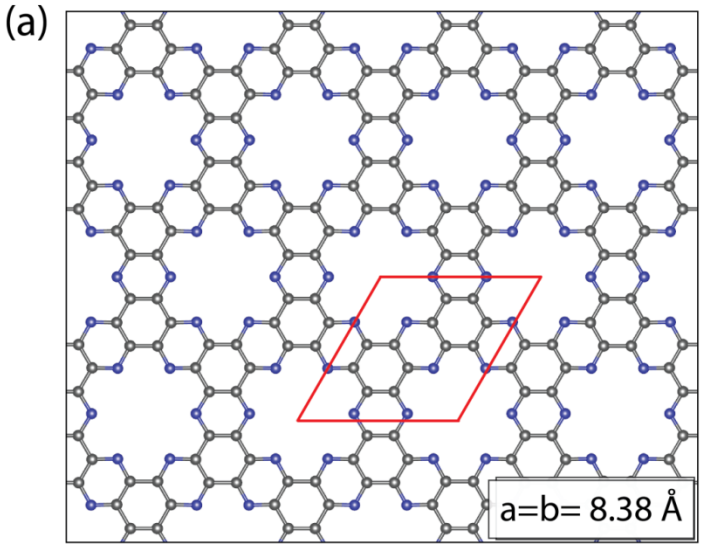
- Synthesized with high crystallinity
- Relatively high carrier moblities
- Promissing material for device applications

J. Mahmood, Jong-Beom Baek,Nat. Commun. 6, 6486, 2015.

Results

2D Hexagonal C_2N COF

Optimized Geometry



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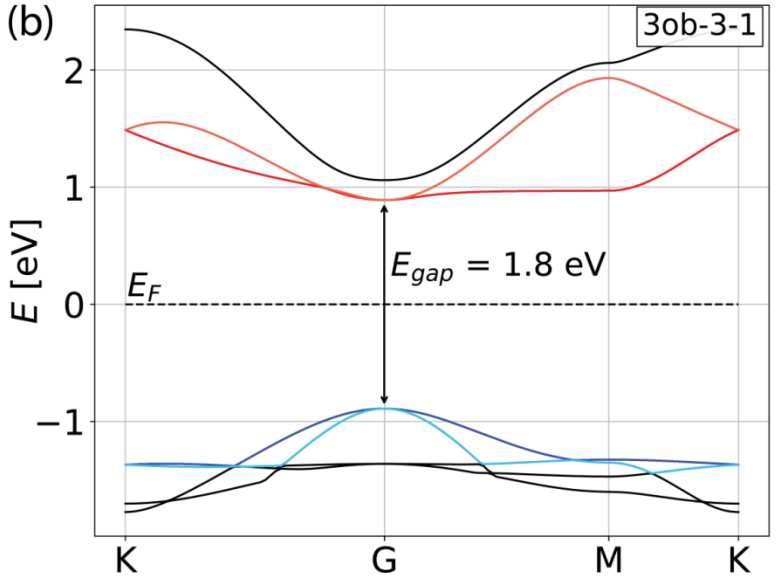

Degeneracy at the band edges
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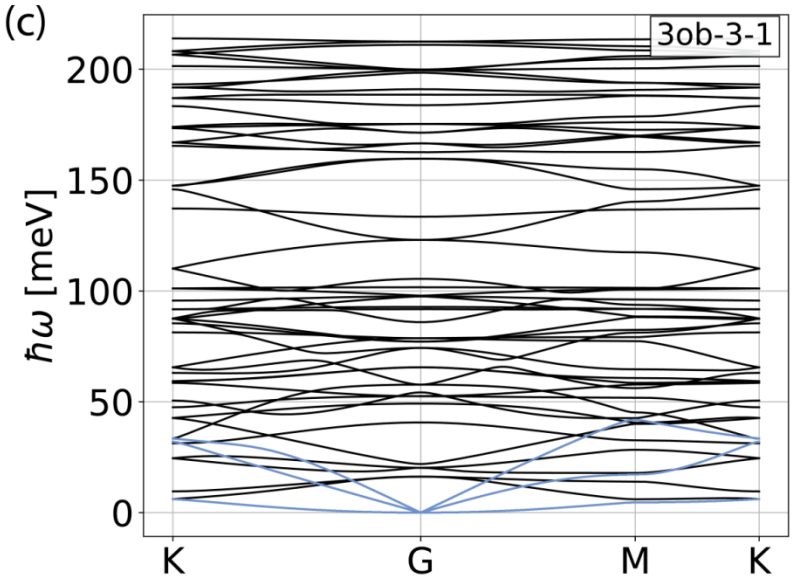
Phononic Properties



Max. phonon freq. up to ≈ 220 meV

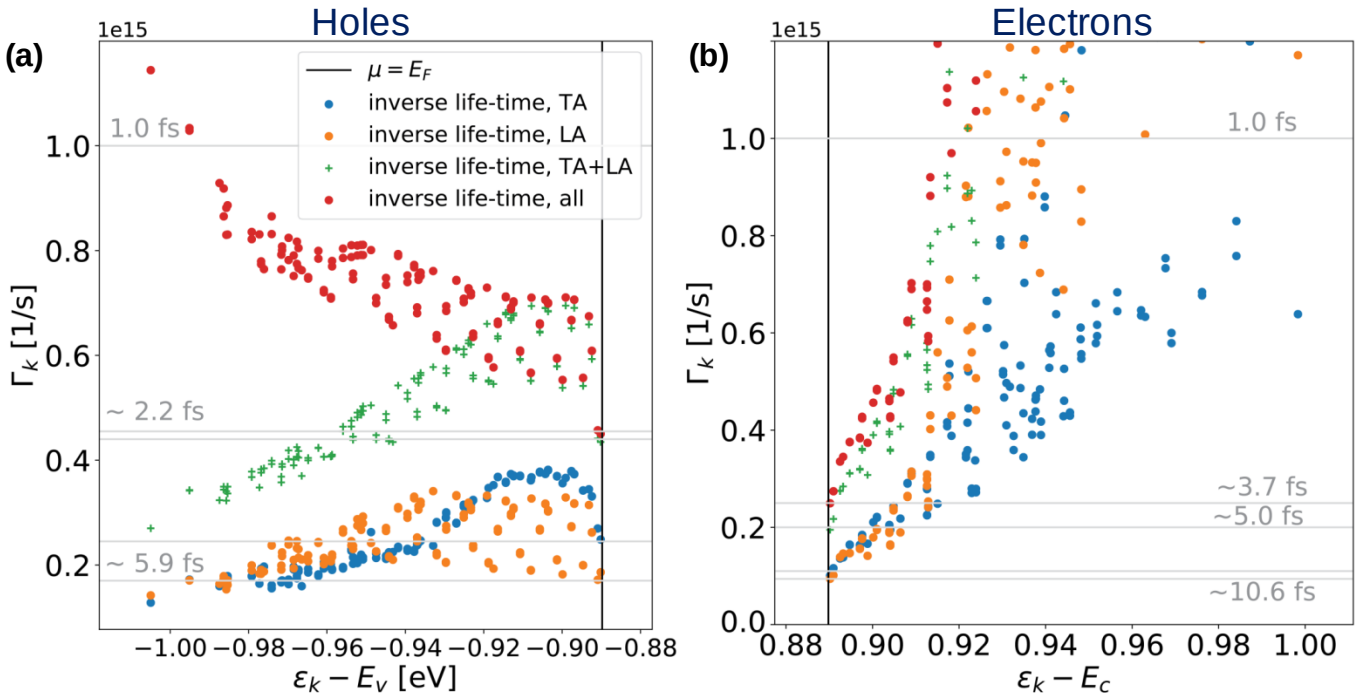
- Synthesized with high crystallinity
- Relatively high carrier moblities
- Promissing material for device applications

J. Mahmood, Jong-Beom Baek,Nat. Commun. 6, 6486, 2015.

Results

2D Hexagonal C_2N COF

Scattering Rates



Results

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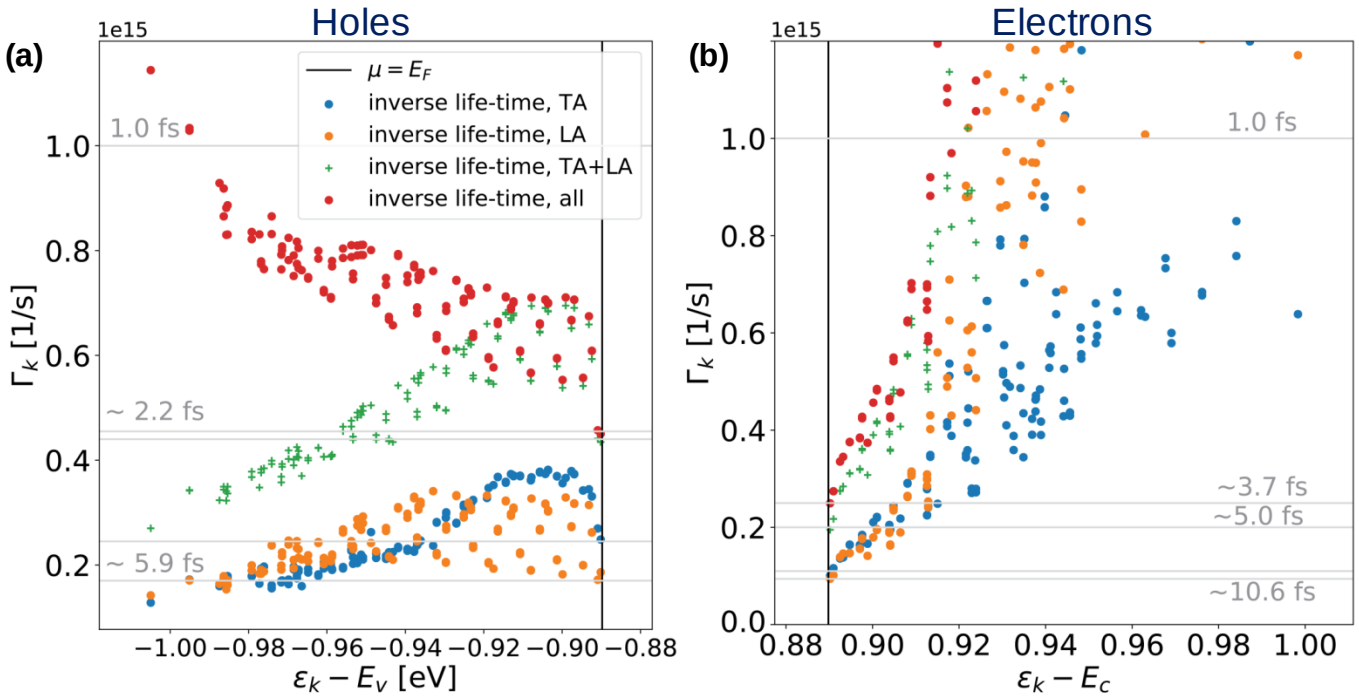
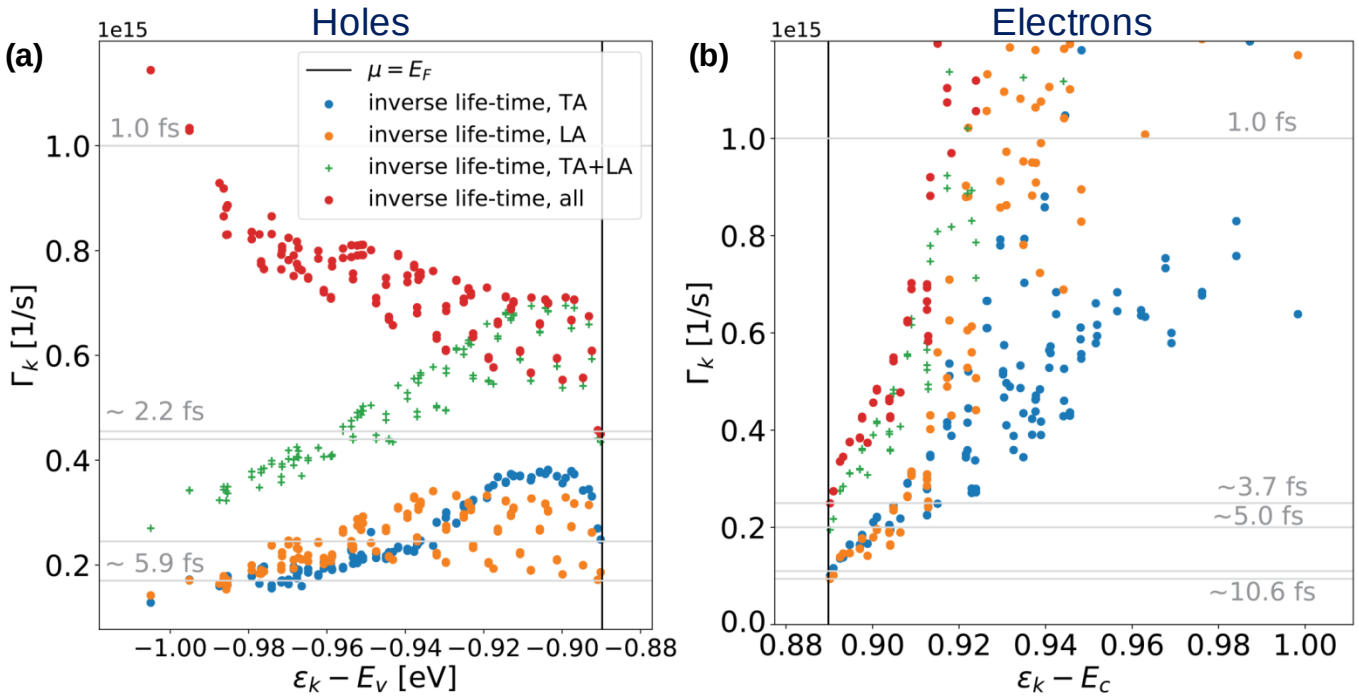


Band edge Acoustic phonon scattering is dominant
τ (Holes) = 2.2 fs
τ (Electrons) = 3.7 fs

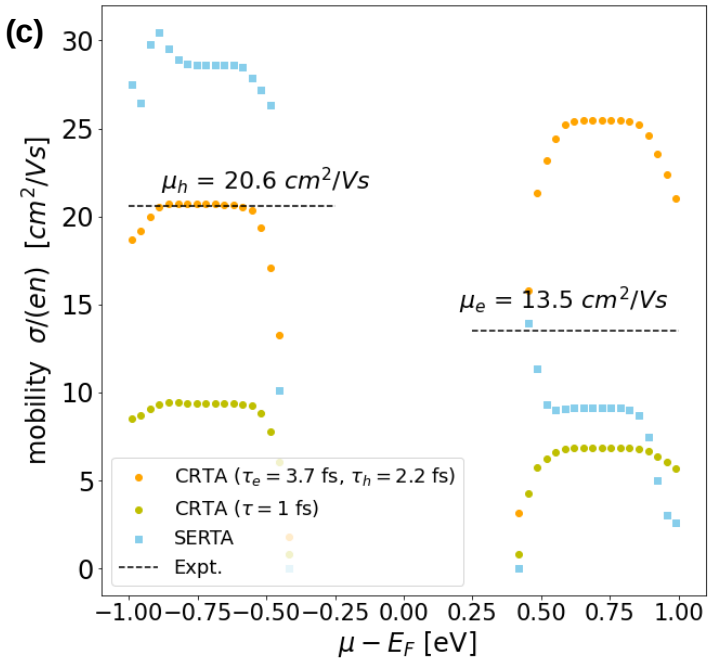
Results

2D Hexagonal C_2N COF

Scattering Rates



Room Temperature Mobilities



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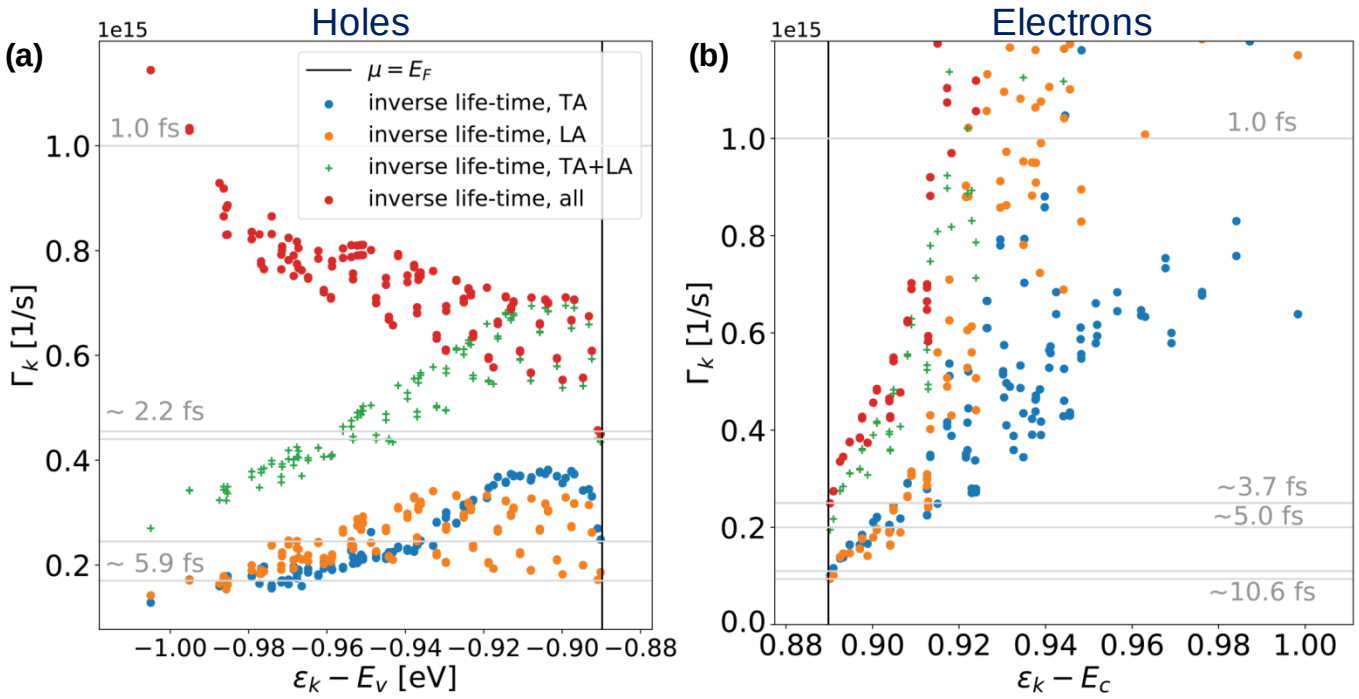
J. Mahmood, Jong-Beom Baek,Nat. Commun. 6, 6486, 2015.

Results

2D Hexagonal C_2N COF

Scattering Rates



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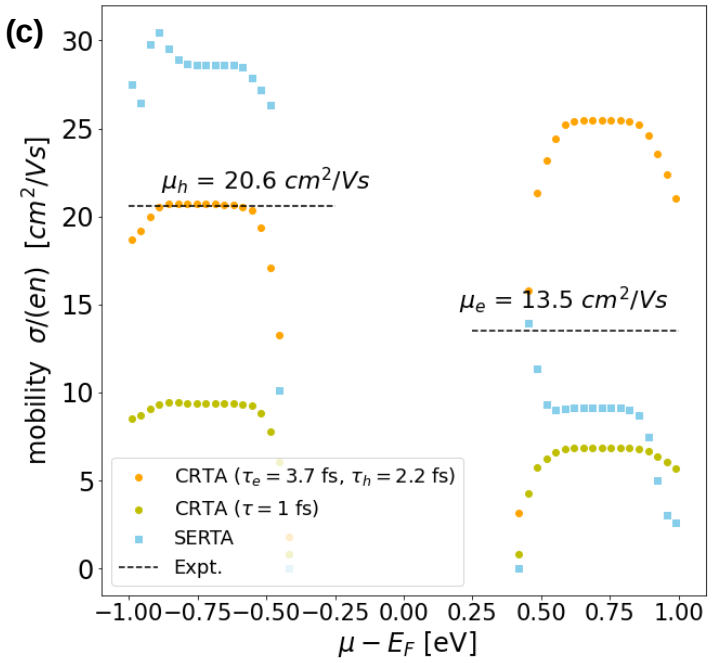


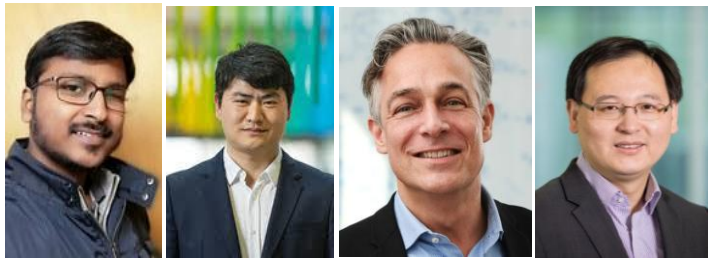
Band edge Acoustic phonon scattering is dominant
τ (Holes) = 2.2 fs
τ (Electrons) = 3.7 fs

τ estimation is important!
Good agreement w/ expt. results!

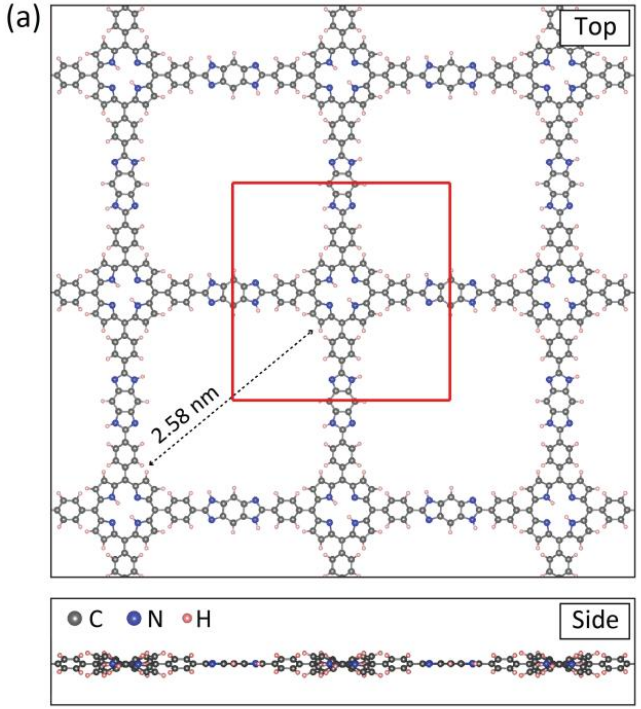
J. Mahmood, Jong-Beom Baek, Nat. Commun. 6, 6486, 2015.

Results

2D Polybenzimidazole COF



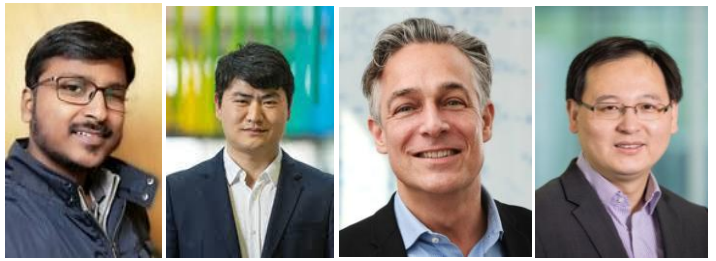
Optimized Geometry



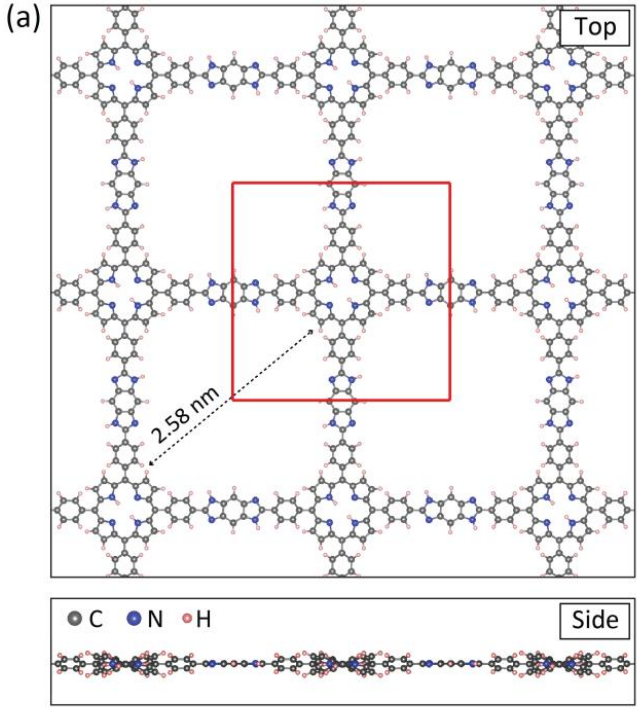
a=2.5 nm
Expt. & Computational

Results

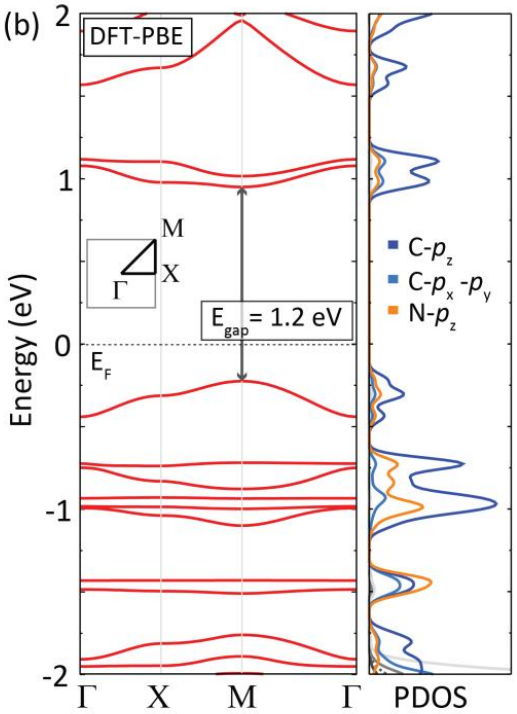
2D Polybenzimidazole COF

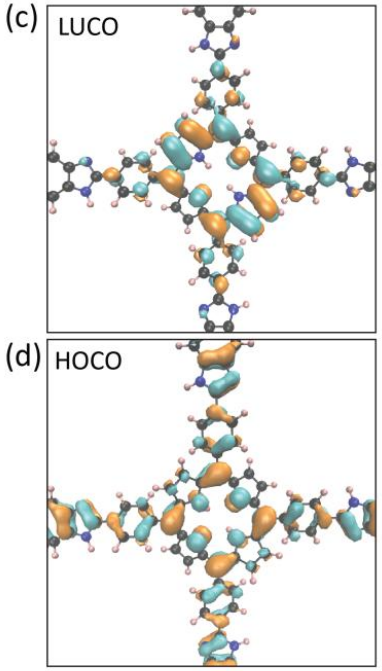


Optimized Geometry



Electronic Properties





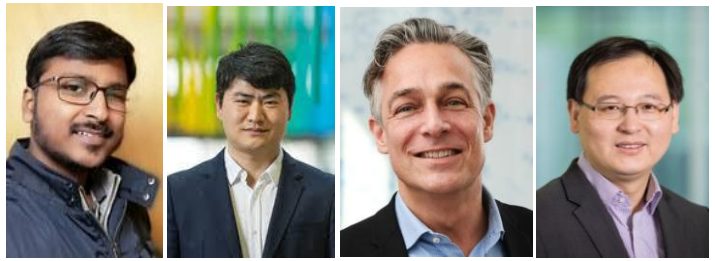
a=2.5 nm
Expt. & Computational

E_{gap}(expt.) = 1.1 eV

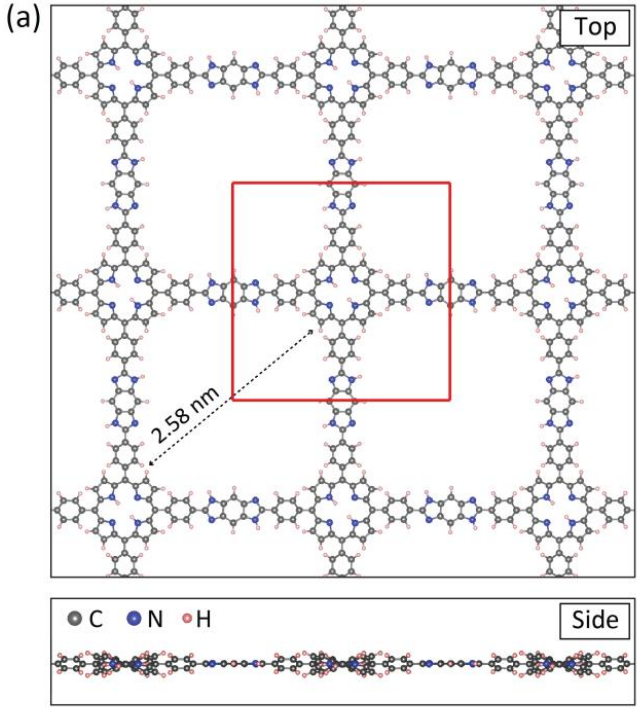
Delocalized holes

Results

2D Polybenzimidazole COF

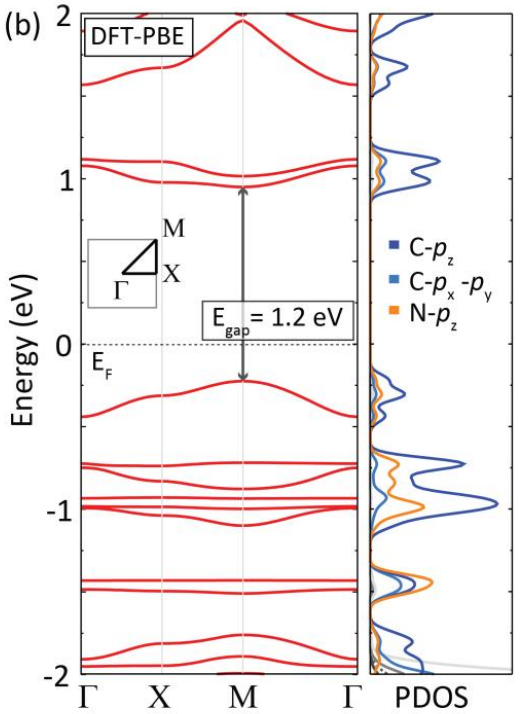


Optimized Geometry

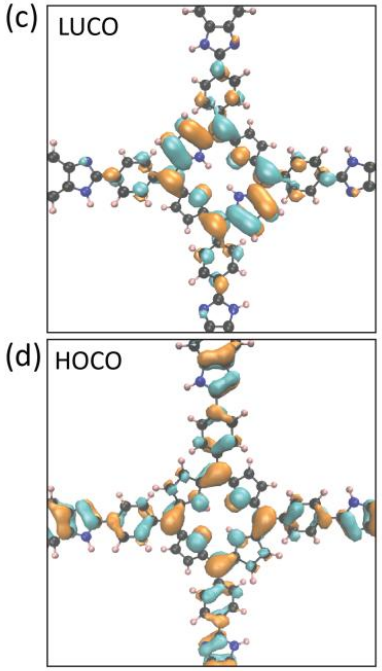


a=2.5 nm
Expt. & Computational

Electronic Properties

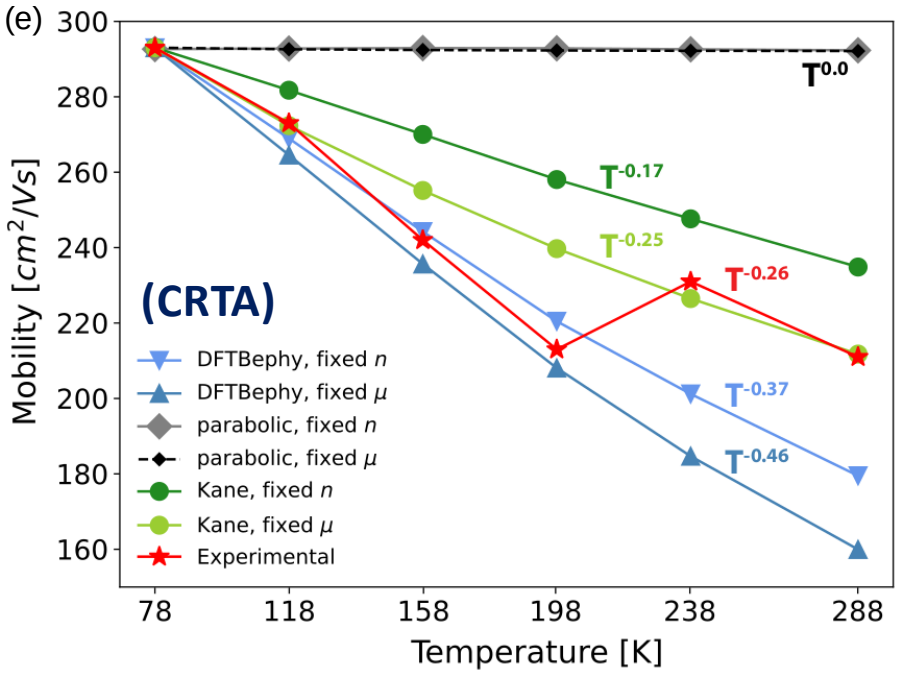


E_{gap}(expt.) = 1.1 eV



Delocalized holes

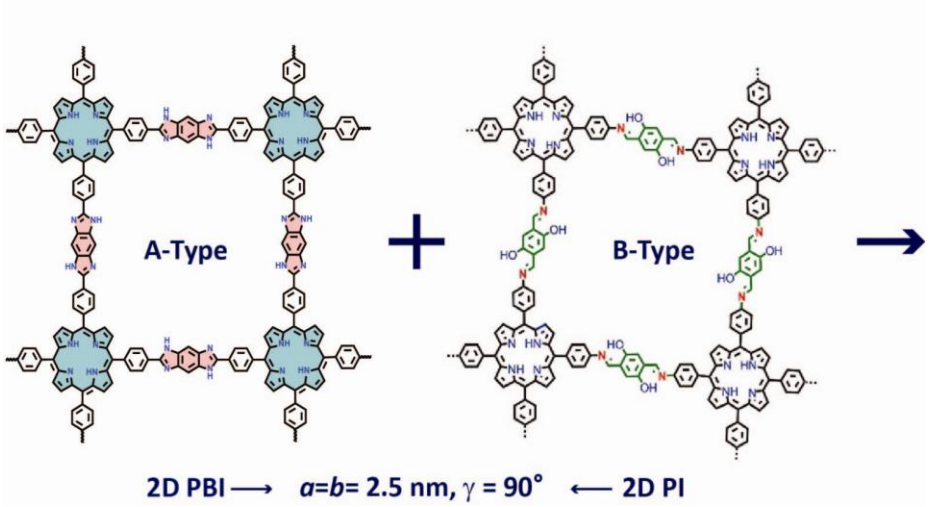
Room Temperature Mobilities



Hole mobilities up to 250 $cm^2V^{-1}s^{-1}$
Good agreement w/ expt. results!

On-going Works

Charge Transport in 2D PBI-Polyimine (PI) Heterostructure



No lattice mismatch!

Synthesized:

- AB-Type
- BA-Type

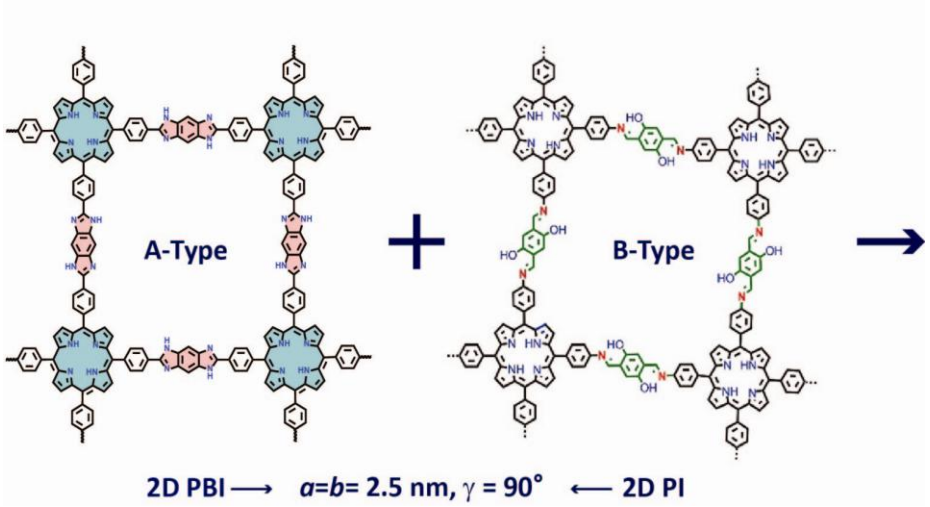
Charge transfer between the layers

In-plane mobility of the heterostructure

- Computational
- Experimental

On-going Works

Charge Transport in 2D PBI-Polyimine (PI) Heterostructure



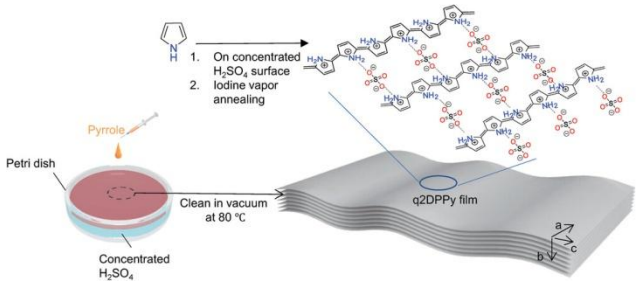
No lattice mismatch!

Synthesized:
- AB-Type
- BA-Type

Charge transfer between the layers

In-plane mobility of the heterostructure
- Computational
- Experimental

SMAIS Method Project-Structural Simulation of Quasi-2D Polyacetylene



Electronic Properties

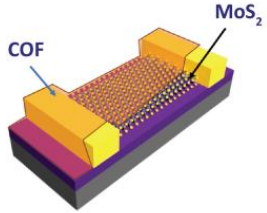
Charge carrier mobility
- Computational
- Experimental

Overview

Publications

- Enhancing the carrier transport in ML MoS2 through interlayer coupling with 2D COFs

  [C.Wang, L. Cusin, C. Ma, E. Unsal, H. Wang, V.G. Consolaro, V. Montes-Garcia, B. Han, S. Vitale, A. Dianat, A. Croy, H. Zhang, R. Gutierrez, G. Cuniberti, Z. Liu, L. Chi, A. Ciesielski, P. Samori, Adv. Mater. 36 (1) 2024]



- DFTBephy: a DFTB-based approach for electron-phonon coupling calculations

  [A. Croy, E Unsal, R. Biele, A. Pecchia, JCEL 22 (5), 2023]

- Introducing cationic surfactant in SMAIS to sythesize a large single crystal domain of 2D PBI polymer (in preparation)

  Collaboration with A. Prasoon, R. Dong, X. Feng

- First-Principles Investigation of Electron-Phonon Couplings in g-Graphyne (in preparation)

  Collaboration with A. Croy and A. Pecchia

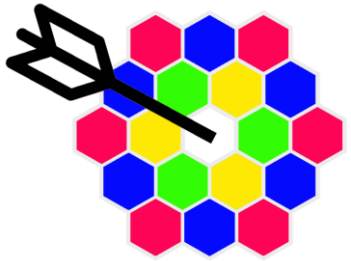
- Theoretical Investigation of Charge Transport in C_2N (in preparation)

  Collaboration with A. Croy and Pecchia

Overview

ULTIMATE Secondments

- @ISIS, UNISTRA (February 14- March 26, 2022)
- @HechtLab, Humboldt University of Berlin (February 14- March 26, 2023)



ULTIMATE meetings

- 6 progress meetings, 2 schools, 3 workshops, symposium

Deliverables

- **D1.1:** Report on modeling the inter- and intramolecular interactions in S2DMs
- **D1.2:** Progress report on design and optimization of S2DMs
- **D1.3:** Report on structural and electronic properties of S2DMs

Milestone

- **MS7** Model and codes for design and optimization of S2DMs

Final Report on Work Package

- **WP1** Design and theory of new functional molecular building blocks (by March 29th, 2024)

Overview

7 Poster Sessions

- Virtual School on Many-Body Calculations using EPW and BerkeleyGW, online (June 9, 2023)
- CRC 1415 Retreat 2023, Niederwiesa, DE (May 9, 2023)
- CECAM Workshop on Quantum Transport Methods and Algorithms, Zurich, CH (July 8, 2022)
- CRC 1415 Retreat 2022, Niederwiesa, DE (June 15, 2022)
- DFTB+ School, Daresbury, UK (June 5-10, 2022)
- 3rd Chem2DMat2021, online (September 1, 2021)
- International Workshop on Charge Transport and Excited State Processes in Organic Materials, online (June 21 2021)

3 Talks

- DPG SKM Spring Meeting, Berlin (March 2024)
- DPG SKM Spring Meeting, Dresden (March 2023)
- DPG SKM Meeting, Regensburg (September 2022)

Overview

Teaching Assistant

- Nanostructured Materials (SoSe23, SoSe22, SoSe21)
- Concepts of Molecular Modelling (WiSe23, WiSe22)

Rigorosum

- Nanostructured Materials
- Theoretical Femtosecond Physics - **Frank Großmann**

OR

- Transport Properties of Emerging Materials in Solid State Physics - **Helena Reichlova**

Thesis submission: May-June, 2024 **Estimated defense date: October-November, 2024**

The 2nd Reviewer of thesis: Publishing OK, NOT related to doctoral work/thesis

- Prof. Artur Cielsieski (*COF/MoS2 paper will not be included in the thesis*)

OR

- Prof. Bernd Plietker

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2.2 Applications
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3.1 Electronic Band Structure
3.2 Density Functional Theory
3.3 Density Functional based Tight Binding
3.4 Relaxation Time Approximation
3.5 Semi-classical Boltzmann Transport
3.6 Transport Properties
4 Results and Discussion
4.1 Benchmarking Electron-Phonon Coupling in 2D Graphene Allotropes: DFPT vs. Small-Displacement Method
4.1.1 Graphene
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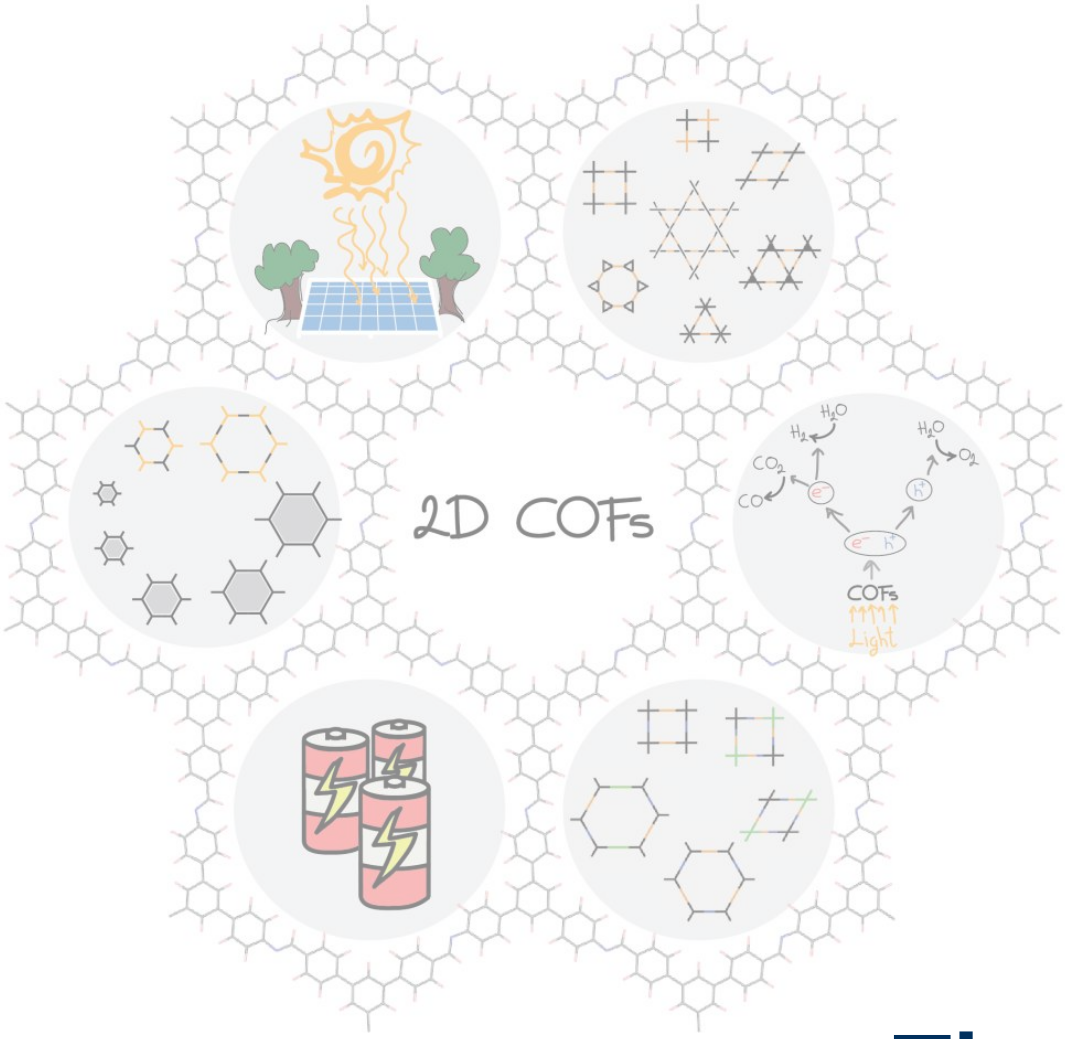
4.2 Metal-free Pyrazine-based COF with High Carrier Mobility: 2D C2N-hex
4.3 Polybenzimidazole COF with High Intrinsic Hole Mobility
4.4 Porphyrin-based COFs (Acoustic Deformation Potential) (?)
4.5 Discussion
5 Summary and Outlook



Thank you for your kind attention!

Backup Slides

DFTBephy: A DFTB-based approach to calculate EPCs

- In-house python package to calculate EPCs using **dftb+** [1] and **phonopy** [2] codes

  https://github.com/CoMeT4MatSci/dftbephy

Boltzmann transport within relaxation time approximation (RTA) [3]:

- Scattering rates within SERTA:

$$\frac{1}{\tau_{m,\vec{k}}} = \frac{2\pi}{\hbar} \sum_{n,\vec{q},\lambda} \left| g^{\lambda}_{nm}(\vec{k},\vec{q}) \right|^2 \left\{ \left[n^0_{\lambda,\vec{q}} + f^0_{n,\vec{k}+\vec{q}} \right] \delta(\varepsilon_{n,\vec{k}+\vec{q}} - \hbar\omega_{\lambda,\vec{q}} - \varepsilon_{m,\vec{k}}) + \left[1 - f^0_{n,\vec{k}+\vec{q}} + n^0_{\lambda,\vec{q}} \right] \delta(\varepsilon_{n,\vec{k}+\vec{q}} + \hbar\omega_{\lambda,\vec{q}} - \varepsilon_{m,\vec{k}}) \right\}$$

- Conductivity within RTA:

$$\sigma_{\alpha\beta} = \frac{e^2}{A_{uc}} \sum_n \int \frac{d^2k}{\Omega_{BZ}} \left[-\frac{\partial f^0(\varepsilon_n(\vec{k});\mu,T)}{\partial \varepsilon} \right] v_{n\alpha}(\vec{k}) v_{n\beta}(\vec{k}) \tau_n(\vec{k})$$

- Mobility:

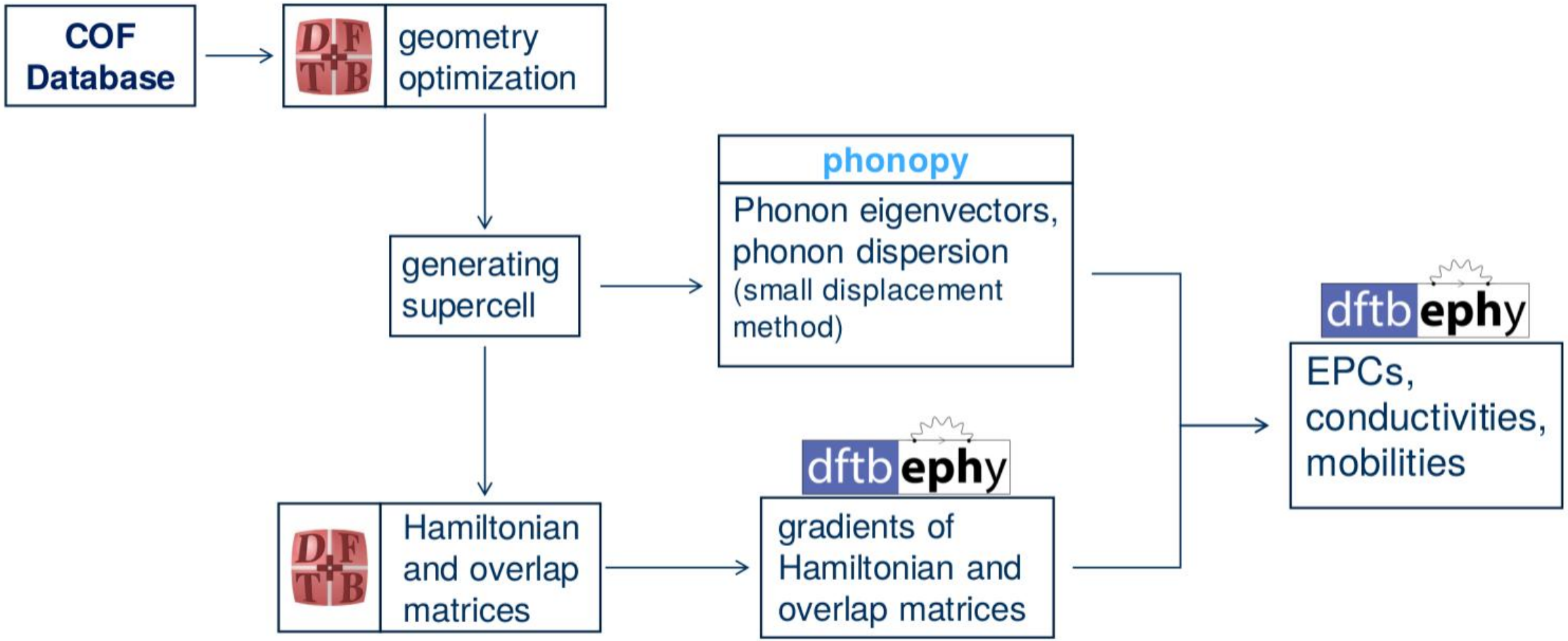
$$\mu_{\alpha\beta}(\mu,T) = \frac{\sigma_{\alpha\beta}(\mu,T)}{e|n_c(\mu,T)|}$$

[1] B. Hourahine et al, J. Chem. Phys. (2020).

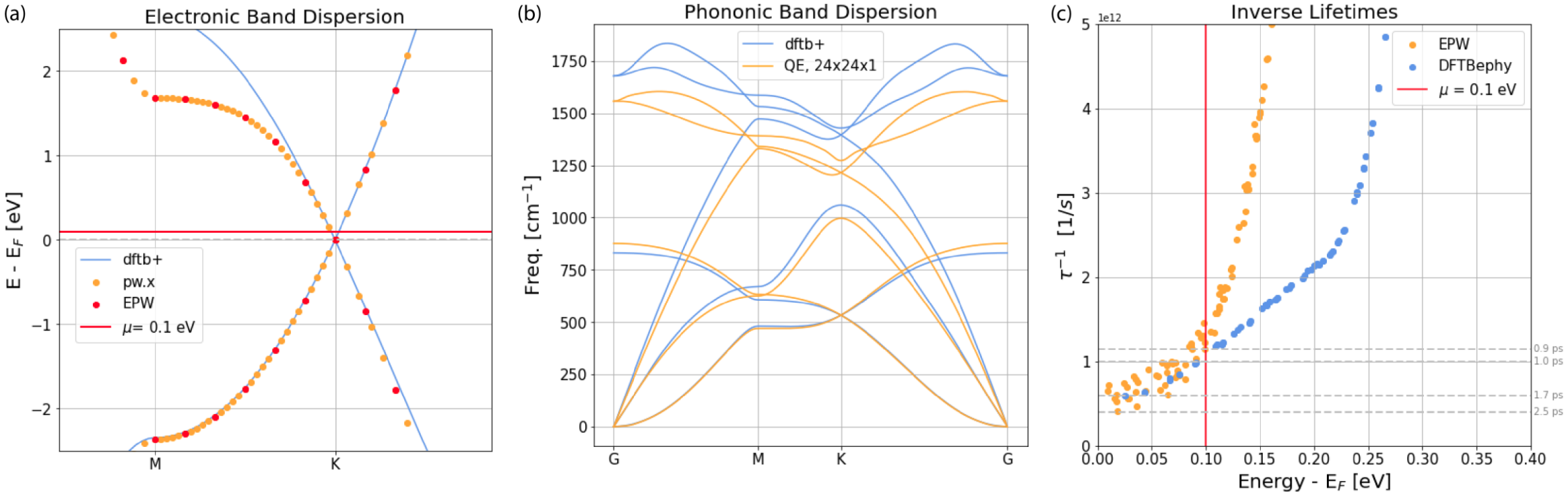
[2] A. Togo and I. Tanaka, Scripta Materialia (2015).

[3] S. Poncé et al, Rep. Prog. Phys. (2020).

DFTBephy: Workflow



Benchmarking Scattering Rates in Graphene: DFTBephy vs EPW



- Scattering rates within SERTA[1]:

$$\frac{1}{\tau_{m,\vec{k}}} = \frac{2\pi}{\hbar} \sum_{n,\vec{q},\lambda} \left| g^{\lambda}_{nm}(\vec{k},\vec{q}) \right|^2 \left\{ \left[n^0_{\lambda,\vec{q}} + f^0_{n,\vec{k}+\vec{q}} \right] \delta(\varepsilon_{n,\vec{k}+\vec{q}} - \hbar\omega_{\lambda,\vec{q}} - \varepsilon_{m,\vec{k}}) + \left[1 - f^0_{n,\vec{k}+\vec{q}} + n^0_{\lambda,\vec{q}} \right] \delta(\varepsilon_{n,\vec{k}+\vec{q}} + \hbar\omega_{\lambda,\vec{q}} - \varepsilon_{m,\vec{k}}) \right\}$$

where EPCs are defined as

$$g^{\lambda}_{nm}(\vec{k},\vec{q}) = \sqrt{\frac{\hbar}{2\omega_{\lambda}(\vec{q})}} \sum_{s,\mu,s',\nu} U^*_{n,s\mu}(\vec{k}+\vec{q}) \left\{ \left[\frac{\partial H_{s\mu,s'\nu}}{\partial \vec{R}_s}(\vec{k}) - \varepsilon_m(\vec{k}) \frac{\partial S_{s\mu,s'\nu}}{\partial \vec{R}_s}(\vec{k}) \right] \frac{\tilde{\mathbf{e}}^{\lambda}_{s}(\vec{q})}{\sqrt{m_s}} - \left[\frac{\partial H_{s\mu,s'\nu}}{\partial \vec{R}_s}(\vec{k}+\vec{q}) - \varepsilon_n(\vec{k}+\vec{q}) \frac{\partial S_{s\mu,s'\nu}}{\partial \vec{R}_s}(\vec{k}+\vec{q}) \right] \frac{\tilde{\mathbf{e}}^{\lambda}_{s'}(\vec{q})}{\sqrt{m_{s'}}} \right\} U_{s'\nu,m}(\vec{k})$$

Non-parabolicity

Non-parabolic bands and carrier mobility

Carrier density:

$$n_C = \frac{m}{2\pi\hbar^2}\int d\varepsilon(1+2\alpha\varepsilon)\frac{1}{e^{(\varepsilon-\mu)/k_BT}+1}$$

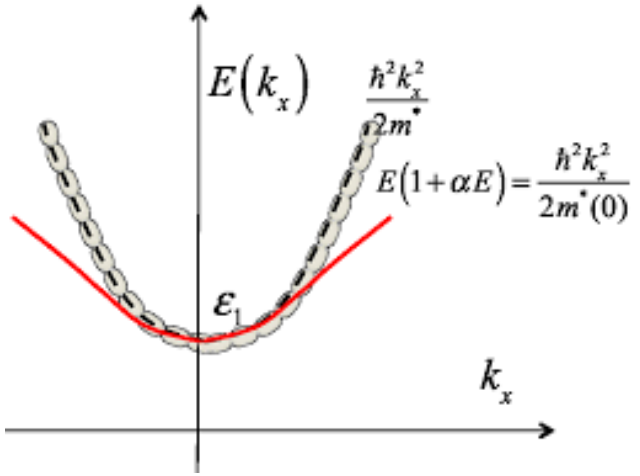
Electrical conductivity:

$$\sigma_{2D} = \frac{e^2}{\hbar^2}\frac{1}{2\pi}\int d\varepsilon\left[\frac{1}{k_BT}\frac{e^{(\varepsilon-\mu)/k_BT}}{(e^{(\varepsilon-\mu)/k_BT}+1)^2}\right]\frac{(\varepsilon+\alpha\varepsilon^2)}{1+2\alpha\varepsilon}\tau_n$$

Mobility:

$$\mu = \frac{\sigma_{2D}}{e|n_C|} = \frac{e\tau_n}{m}\left[\frac{F_0(n)-\alpha k_BT2F_1(n)-2\alpha^2(k_BT)^2 3F_2(n)}{[F_0(n)+2\alpha k_BTF_1(n)}\right]$$

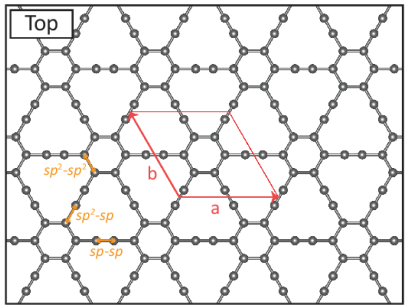
In the parabolic band limit as $\alpha \to 0$, with constant τ_n $\longrightarrow$ **T^0**

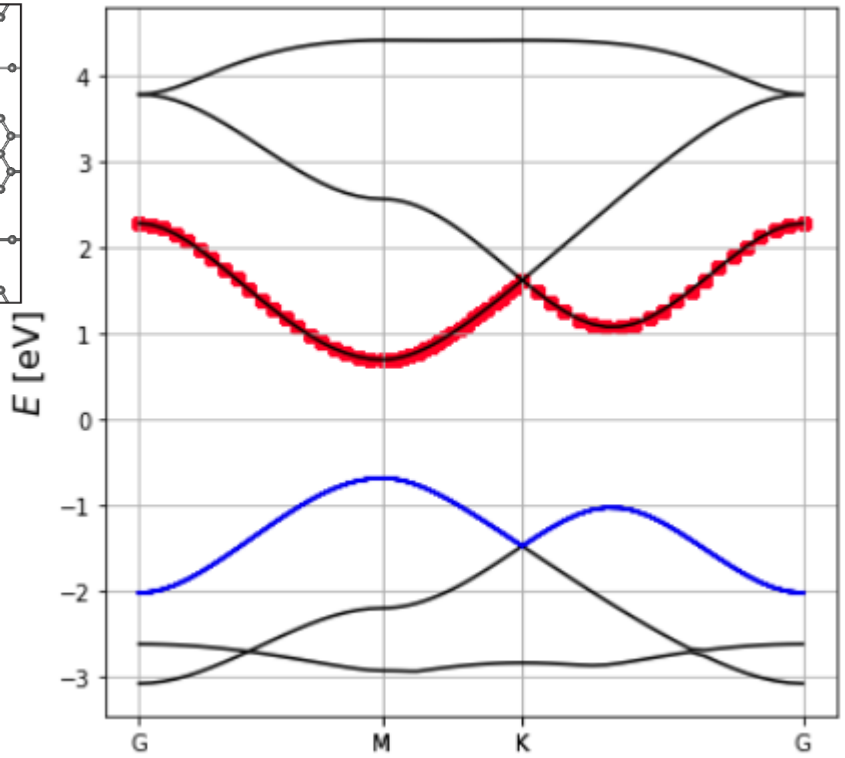


A. M. Ganose et al. 2022, arXiv:2210.01746 [cond-mat.mtrl-sci]

Graphene 2D Allotropes: Electronic Bands

γ-Graphyne



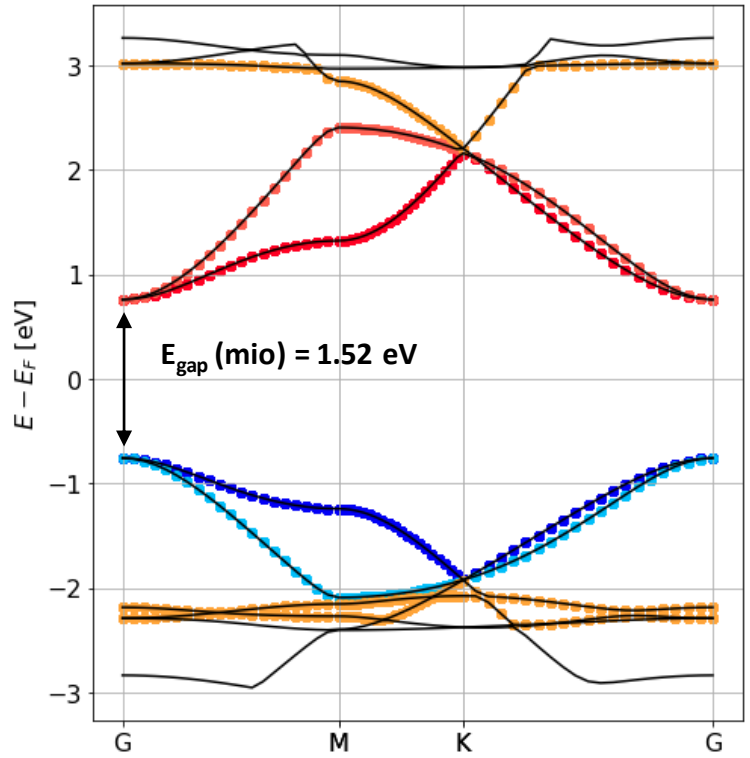


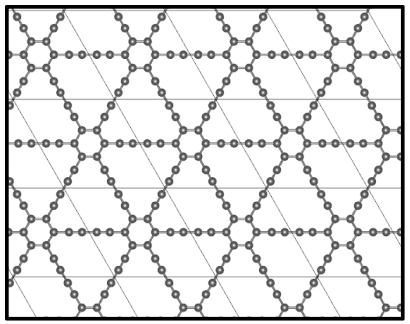
E_{gap} (mio) = 1.38 eV

E_{gap} (PBE) = 0.46 eV

Graphdiyne (GDY)

band gap= 1.5167 eV
EF= -4.847759 eV





E_{gap} (PBE) = 0.48 eV

E_{gap} (HSE06) = 1.11 eV

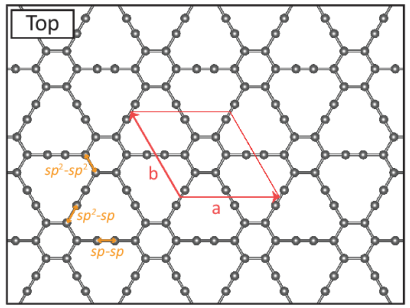
E_{gap} (PBE0) = 1.63 eV

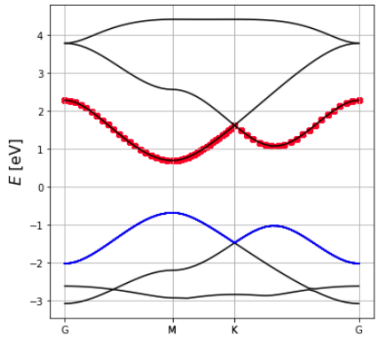
Shuai Group

Results

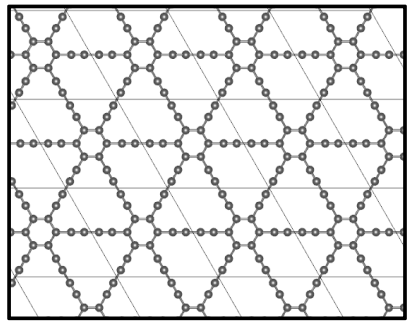
2D Graphene Allotropes: Room Temperature Mobilities w/ CRTA

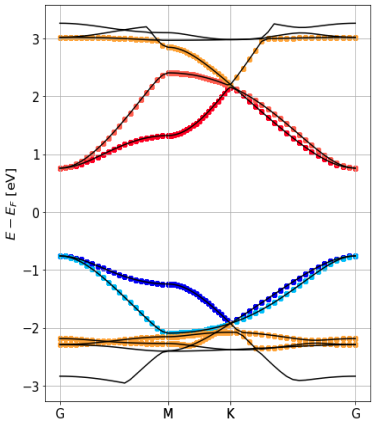
γ-Graphyne

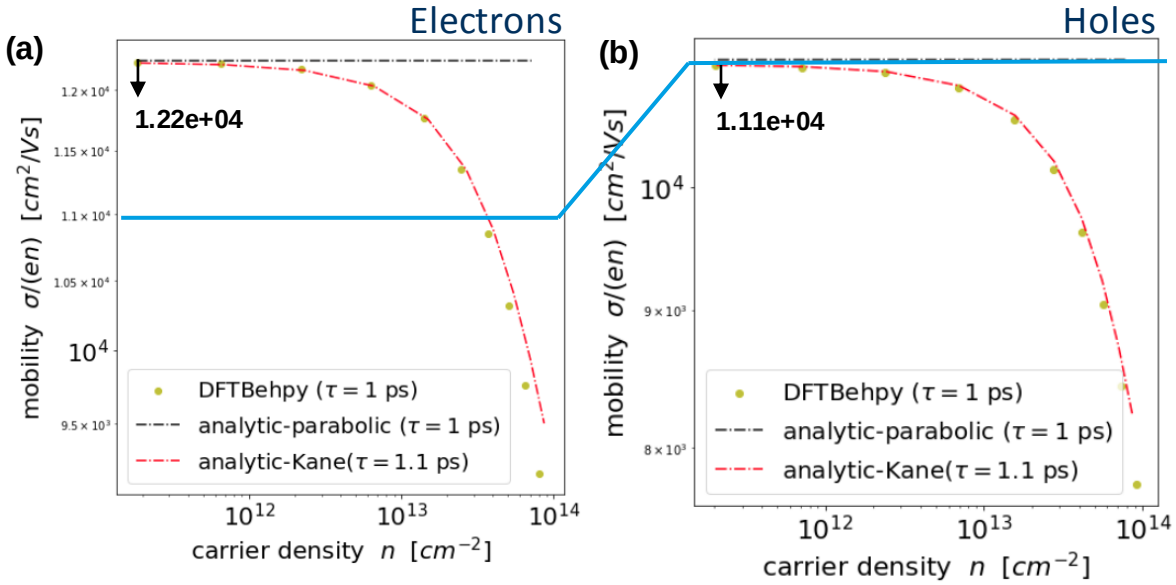


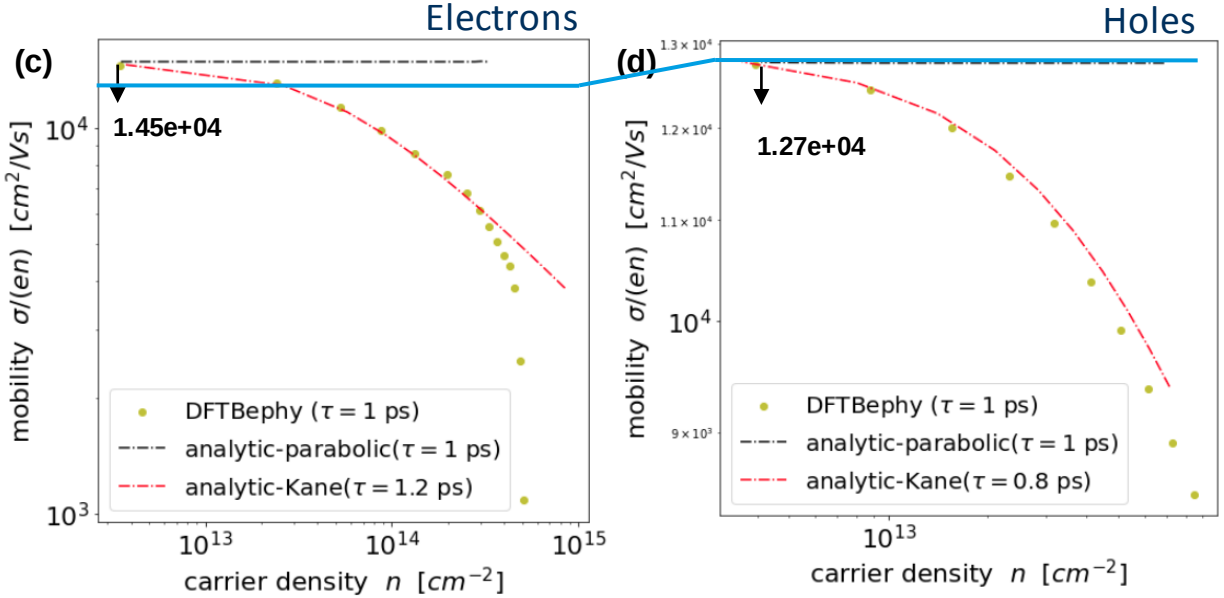


Graphdiyne (GDY)









TOC- Methodology

3 Methodology

3.1 Electronic Band Structure . . . .
3.2 Density Functional Theory . . . .
3.2.1 Kohn-Sham Equations . . . .
3.2.2 Exchange-Correlation Functionals . . . .
3.3 Density Functional based Tight Binding . . . .
3.3.1 Tight Binding . . . .
3.3.2 From DFT to DFTB . . . .
3.3.3 Parametrization . . . .
3.4 Relaxation Time Approximation . . . .
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3.5 Semi-classical Boltzmann Transport . . . .
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3.5.2 Solving the BTE in the Relaxation Time Approximation
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