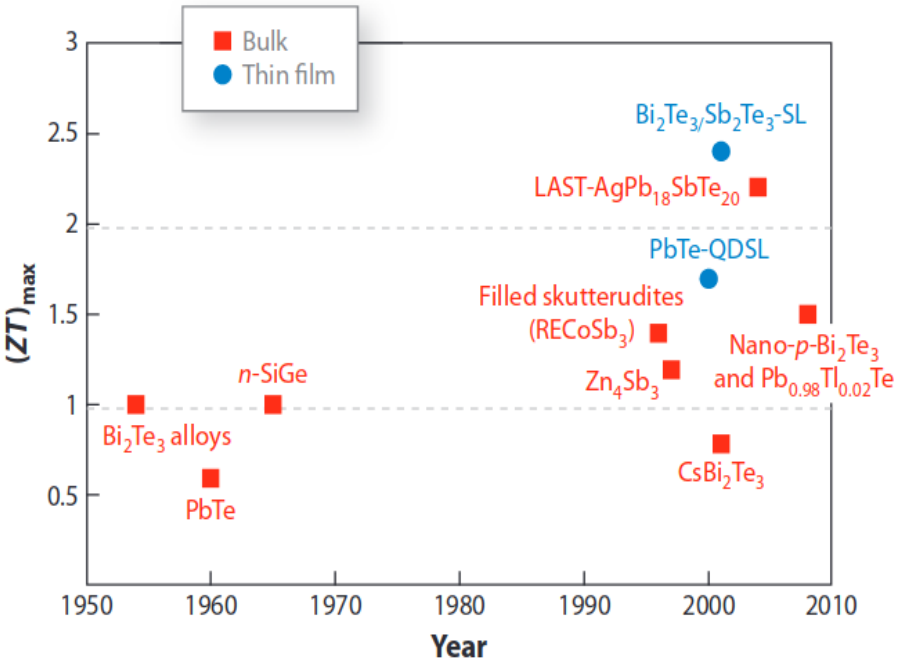
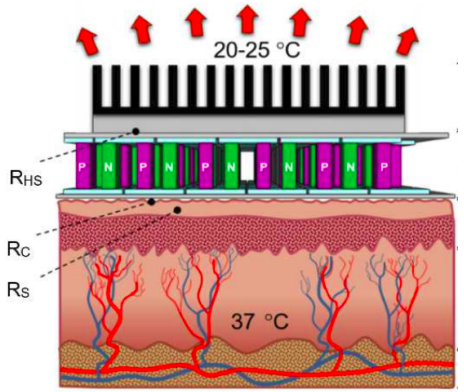
M. Sc Alvaro Gaspar Rodriguez Mendez
IMPRS-TU Dresden

Engineering Transport Properties in Low Dimensional Materials

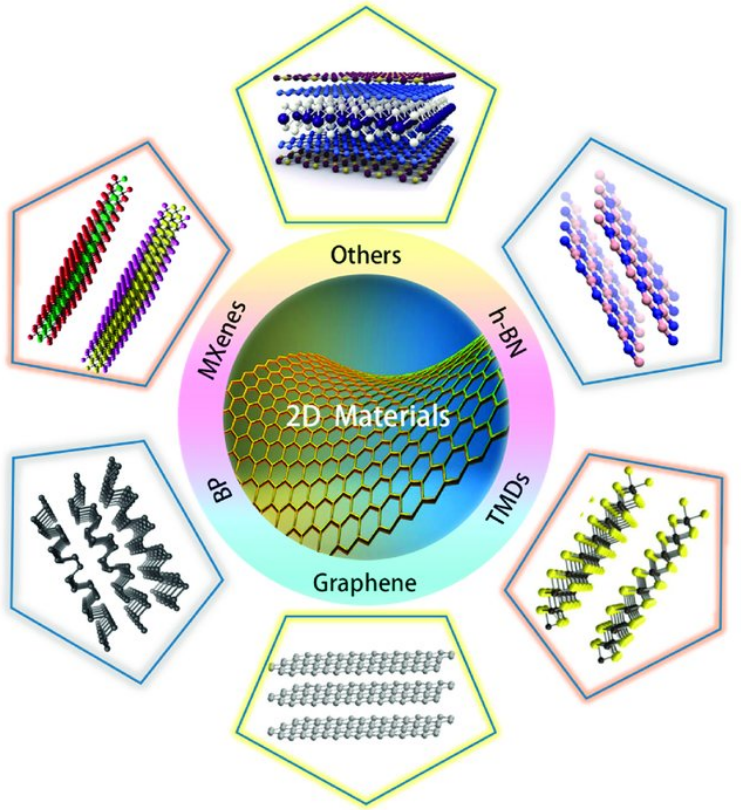
Dresden, January 19th 2020

Motivation



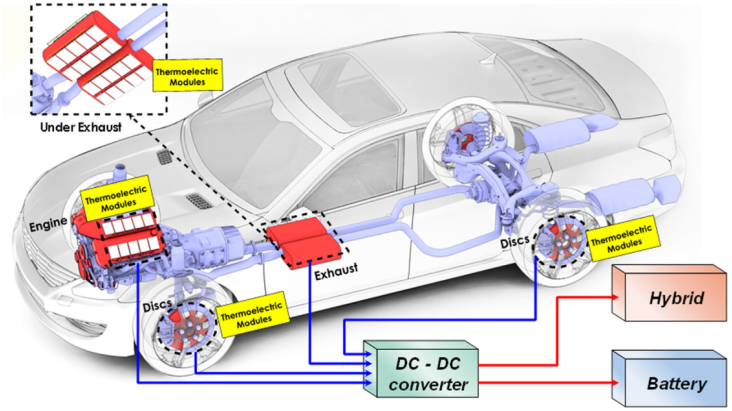


Amin N. et. al. Nano En. 104265 (2019)



Dominance of heavy metals in TE:

- High cost
- Reduced availability
- Toxicity



Dimensionality reduction towards the nanoscale could open a fully new route to optimize the figure of Merit.

Terry T. Annu. Rev. mater. Res. 41, (2011)

Vahid A. et al, Measurement 107035 (2020)

Dresselhaus M. et al. Phys Rev. B 47 (1993)

PhD timeline

Quick-off meeting

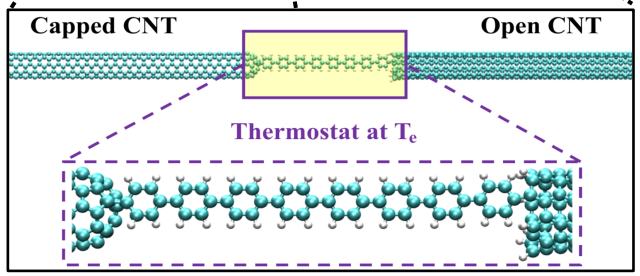
1st TAC meeting

2nd TAC meeting

Jan. 2019

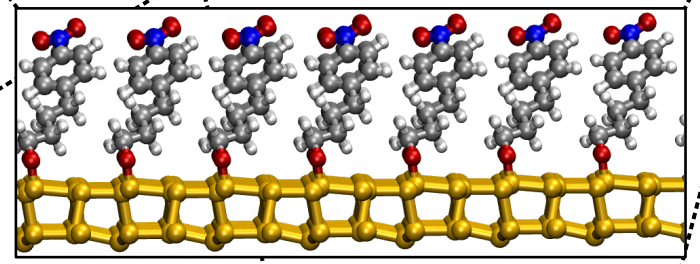
Jan. 2020

Jan. 2021



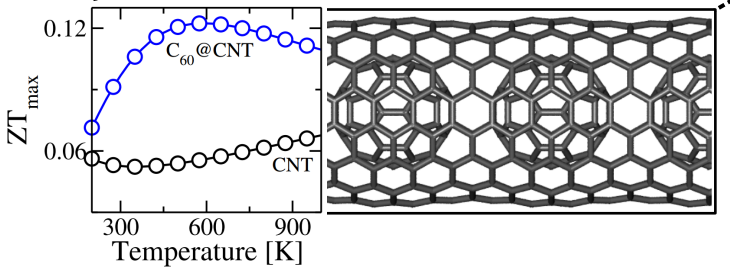
A nanoscale phononic analogue of the Ranque-Hilsch vortex tube. Accepted in PRA2021

Large-scale Hamiltonian and geometry builder for phosphorene w/ wo defects [script].



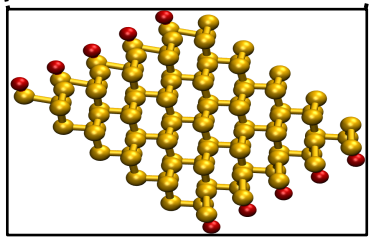
Phosphorene SAM's

CNT-based systems



A Computational Study of the Thermoelectric Signatures of CNT peapods. To be subbmited to JMCC 2021

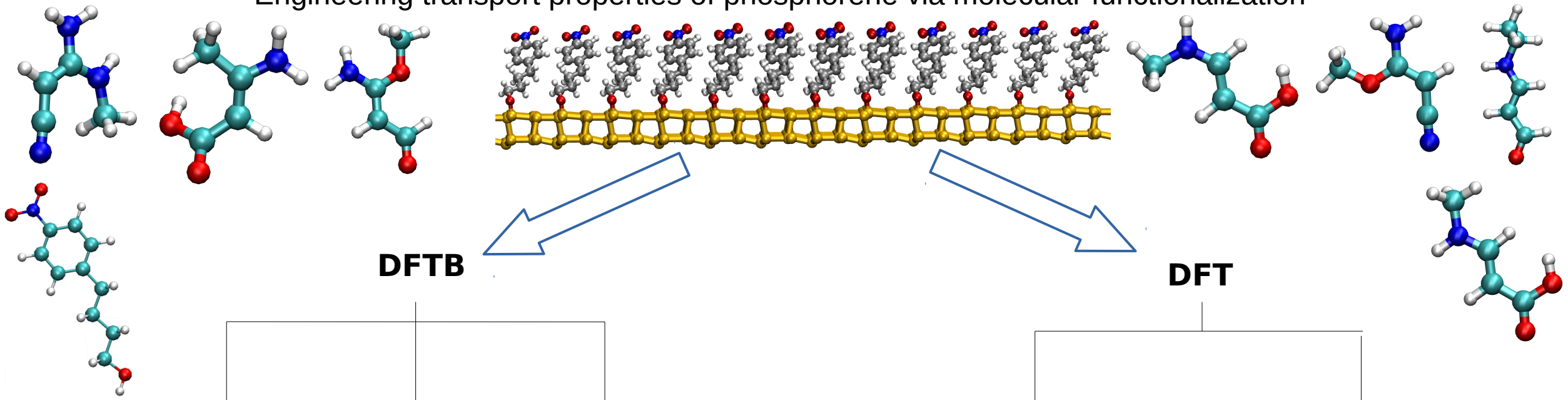
Phosphorene-based systems



Phosphorene Nanoribbons

Self-Assembled Monolayers in Phosphorene

Engineering transport properties of phosphorene via molecular functionalization



DFTB

- Electronic structure
- Density of States
- Electrostatic potential

DFT

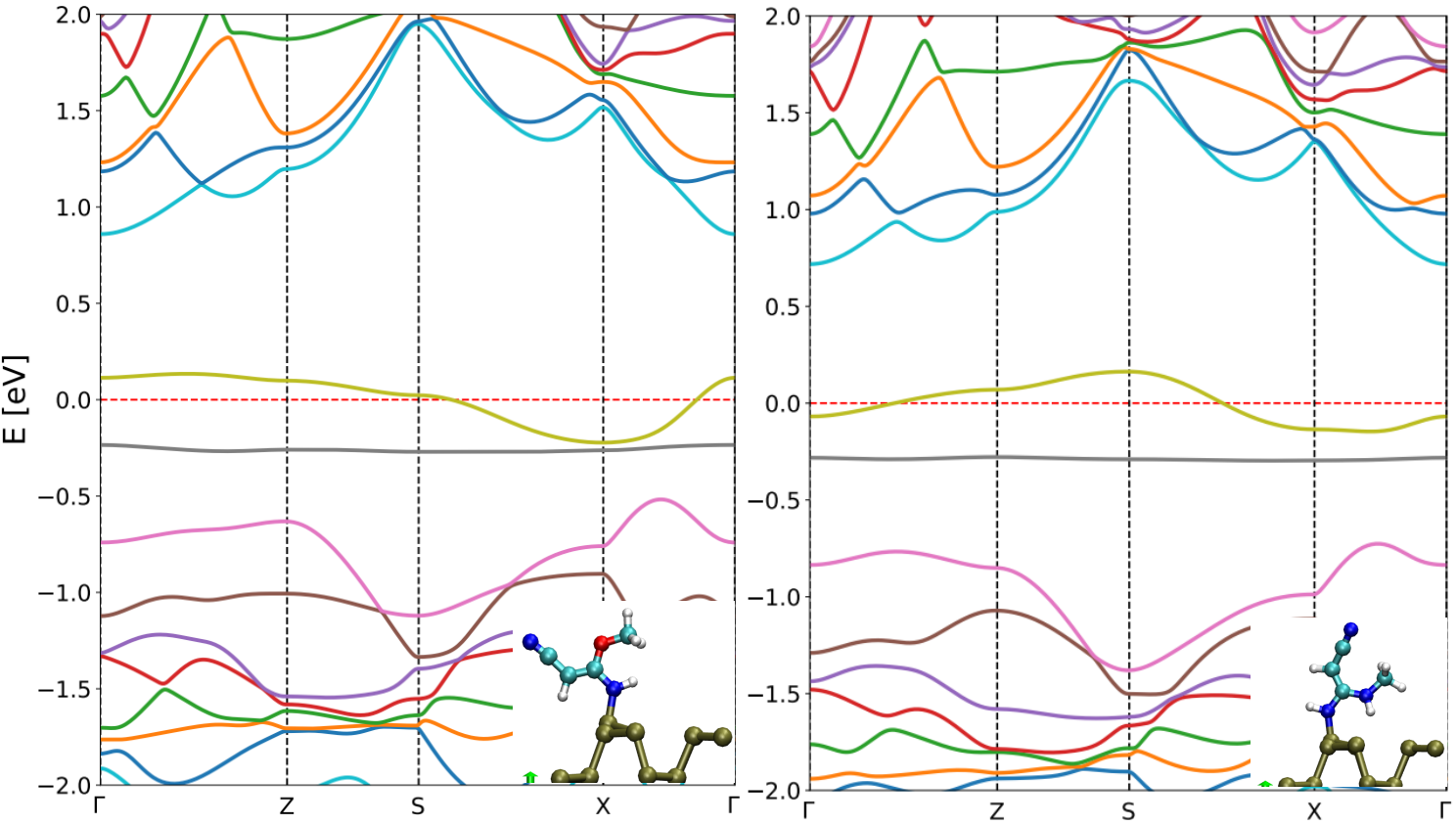
- Electronic structure
- Density of States

- *Electrostatic potential implemented in DFTB+ did not suit the calculation*
- *Geometry optimization of some systems was not accurate*

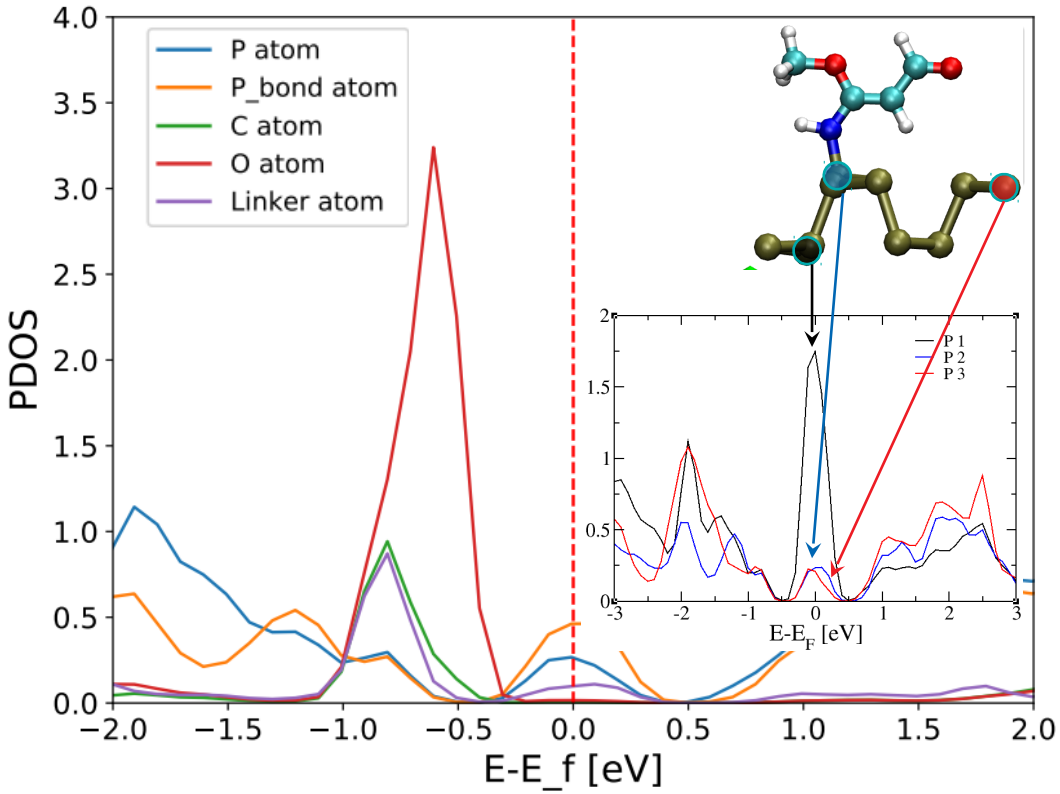
QUANTUMESPRESSO

Self-Assembled Monolayers in Phosphorene

Engineering transport properties of phosphorene via molecular functionalization



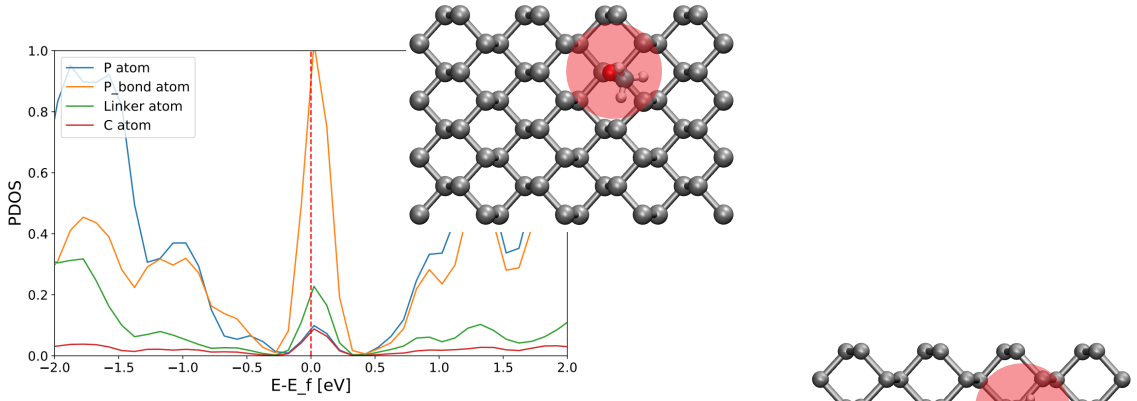
Same atom-type linker between phosphorene and molecule do not produce a big difference in electronic structure (BS/ DOS)

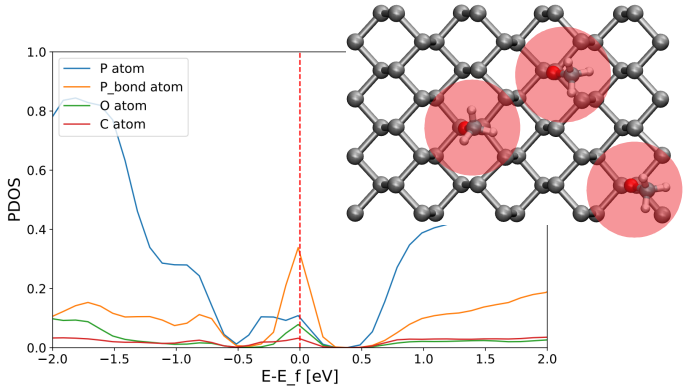


Major contribution around Fermi level comes from unbounded P atoms.

Self-Assembled Monolayers in Phosphorene

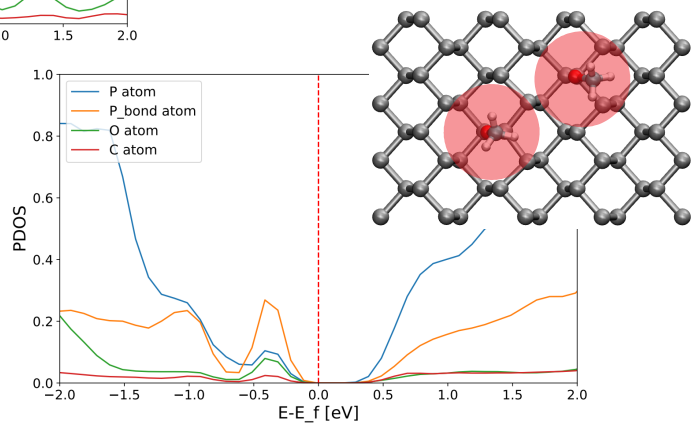
Engineering transport properties of phosphorene via molecular functionalization

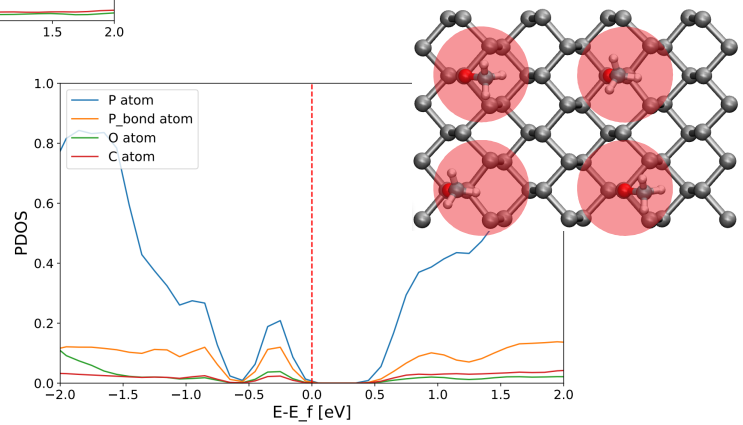




States around Fermi Level

States close to Fermi level





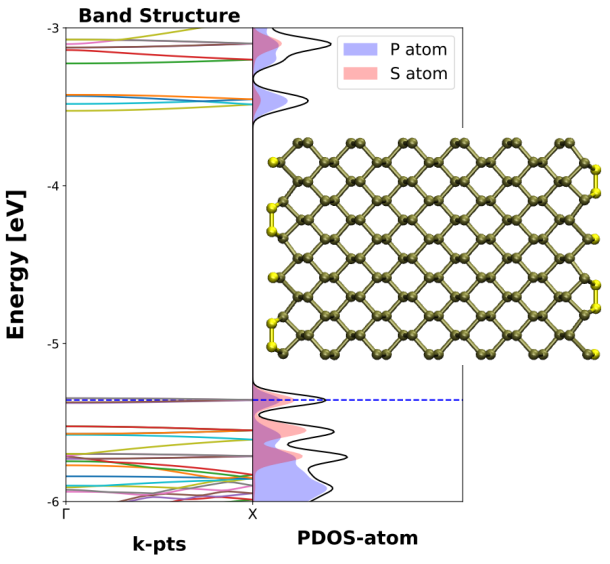
Further steps:

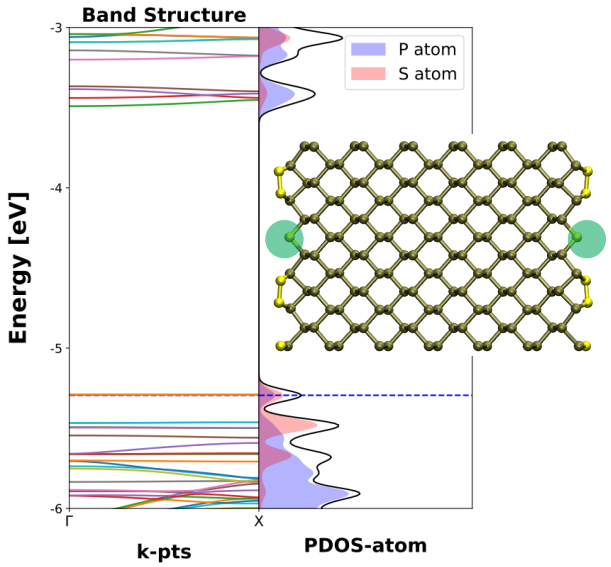
- Further understand the effect of molecular functionalization of phosphorene.
- Compute electronic transport in SAM's based devices (Boltzmann and Landauer).
- Transport properties based on conformational design of device (bilayer, heterolayers, sandwich system).

Defects in x-passivated phosphorene nanoribbons

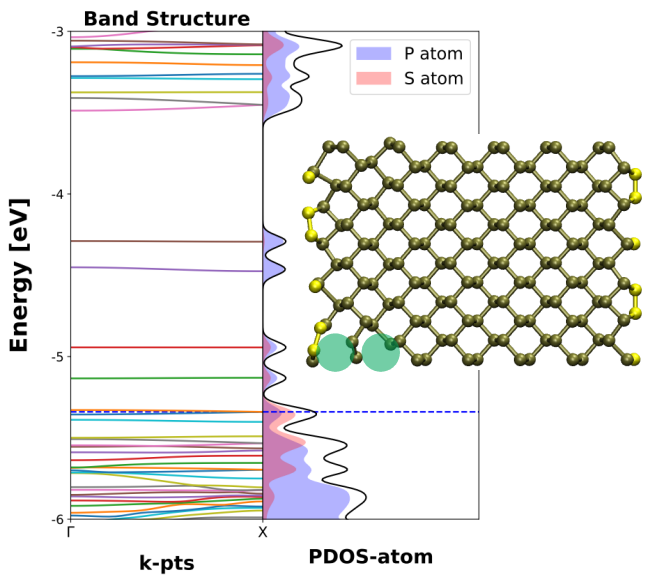
Electronic structure study of **Transport direction** (Zigzag, Armchair), **Atom-type passivation** (H, O, S) and **Vacancies** (MV's, Multiple MV's)

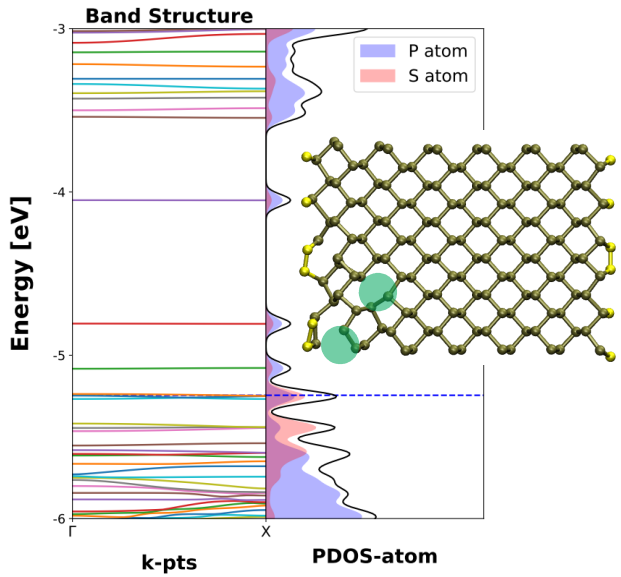
PNR-S pristine





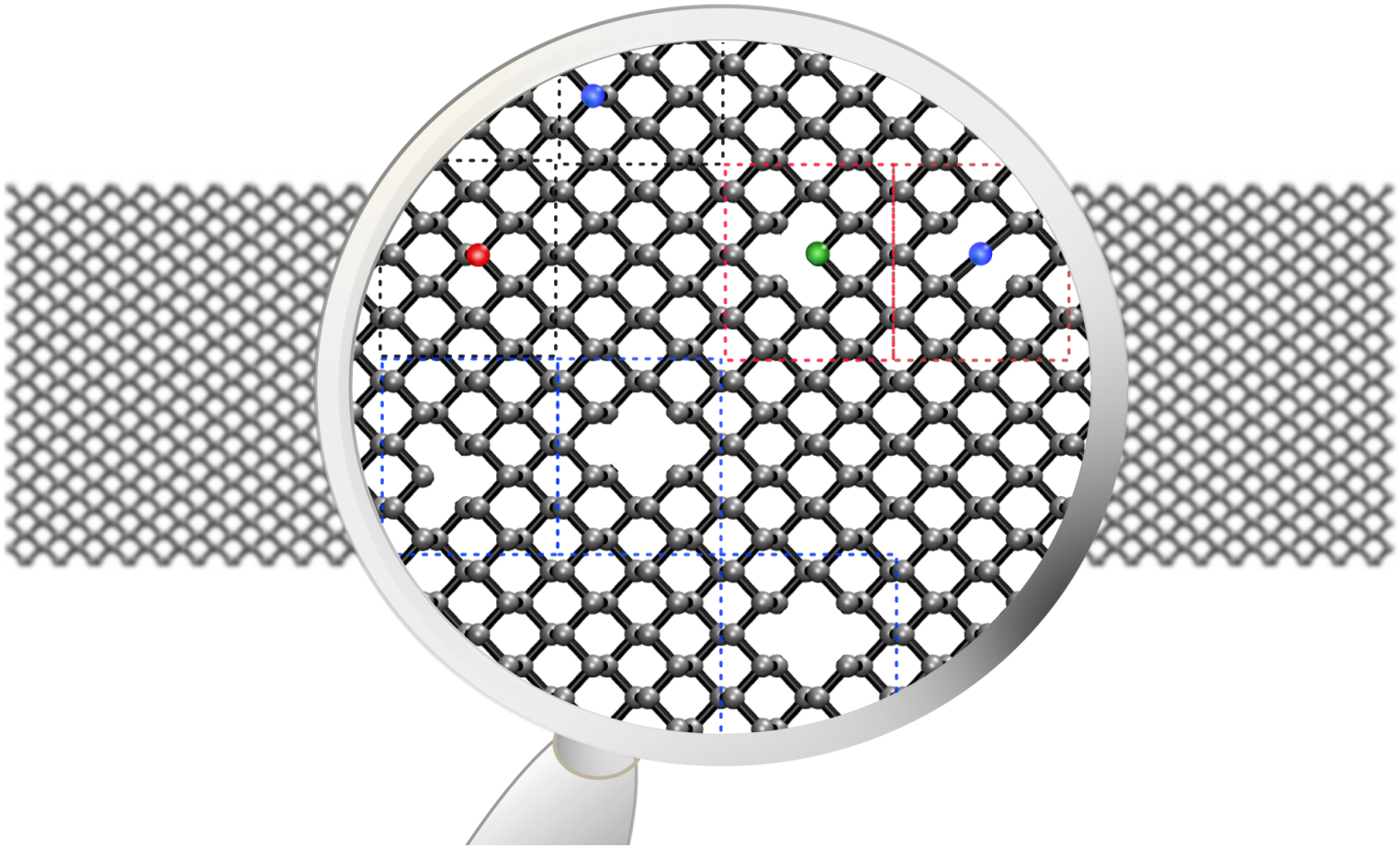
PNR-S with 2 monovacancies





Further steps:

- Compute transport in large scale systems with random location of defects.
- Add strain effect in electronic transport



Additional tasks besides PhD project

T.A. for Nanostructured Materials (summer term) and Concepts of Molecular Modeling (winter term).

PhD goals for the next months...

- Complete electronic transport for defects and passivated PNR systems and prepare paper.
- Prepare paper in molecular functionalization of phosphorene (SAM's).
- Take examination of the "additional courses" as a requirement of PhD enrollment in the faculty.