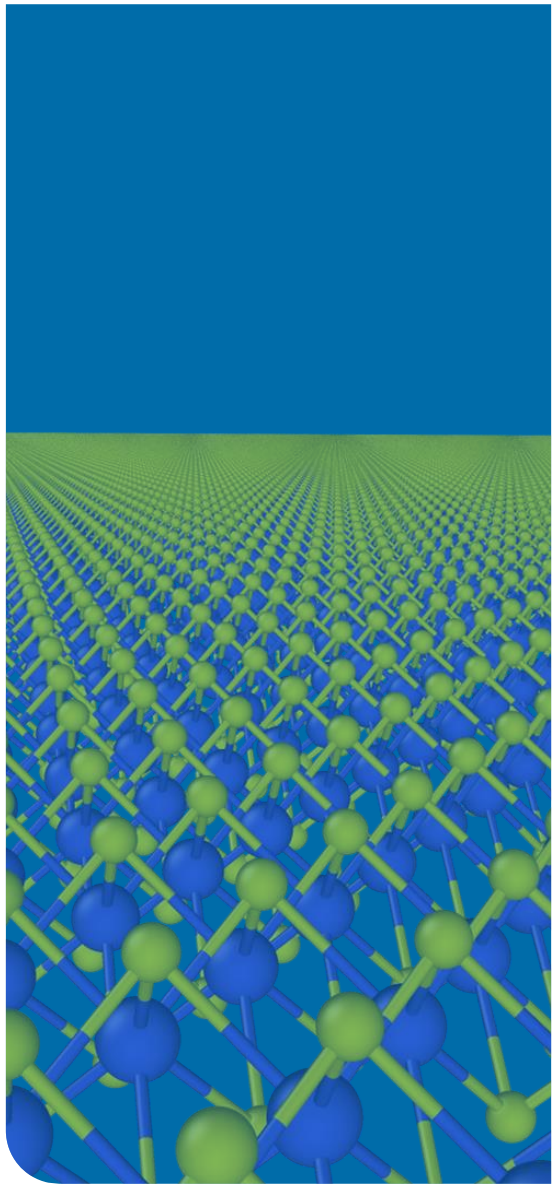
University of Antwerp
CMT | Condensed Matter Theory

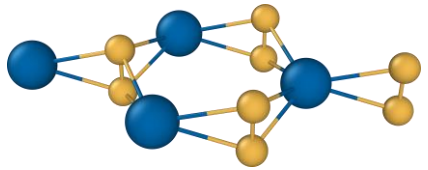
Describing Strain in TMDs using Tight-Binding models

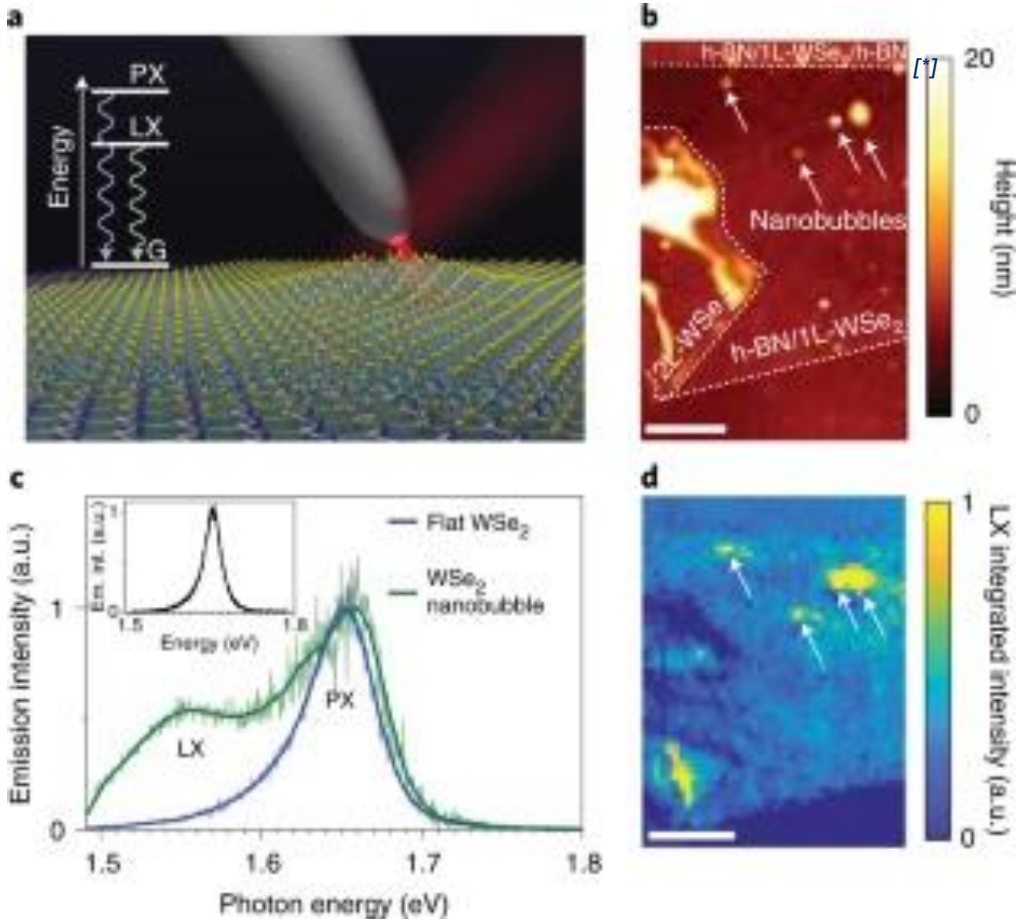
Capri Spring School 2022

Bert Jorissen

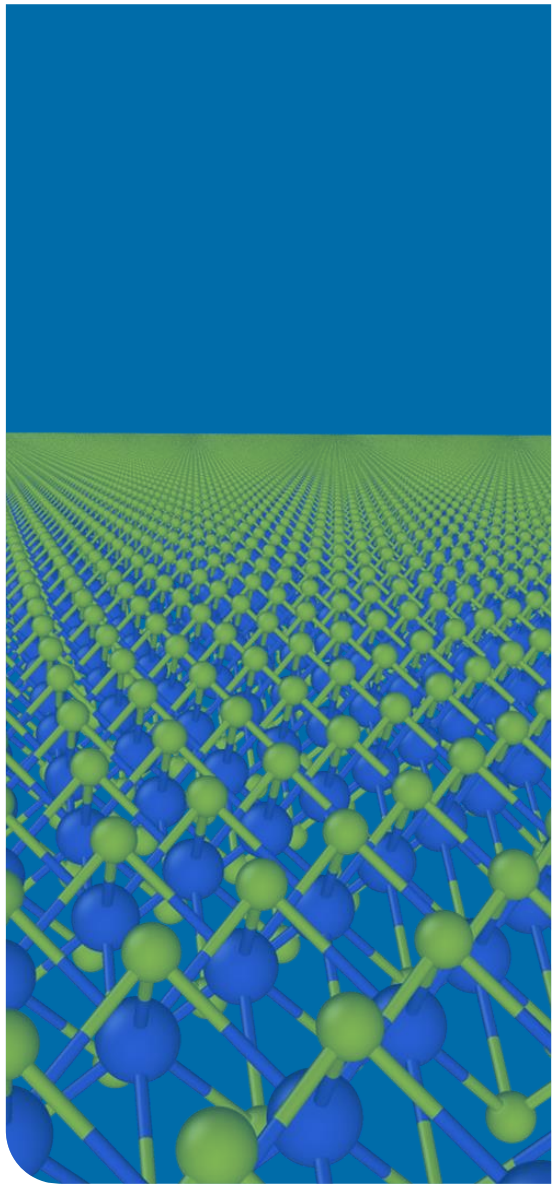


Transition Metal Dichalcogenides

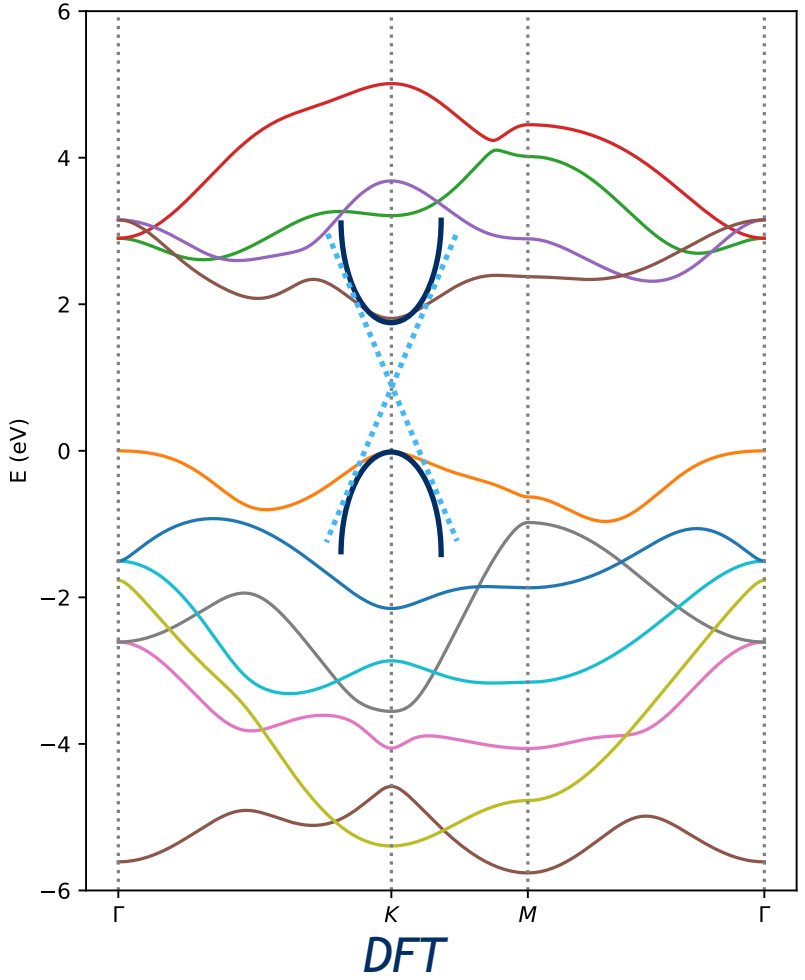




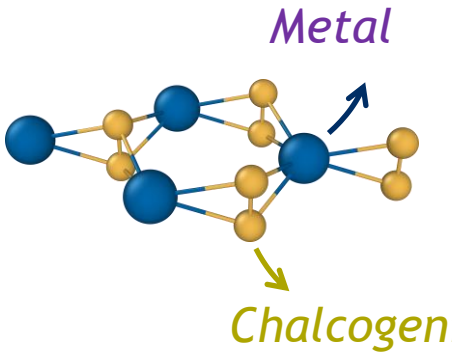
[*] Darlington, T.P., Carmesin, C., Florian, M. et al. Imaging strain-localized excitons in nanoscale bubbles of monolayer WSe2 at room temperature. Nat. Nanotechnol. 15, 854-860 (2020).

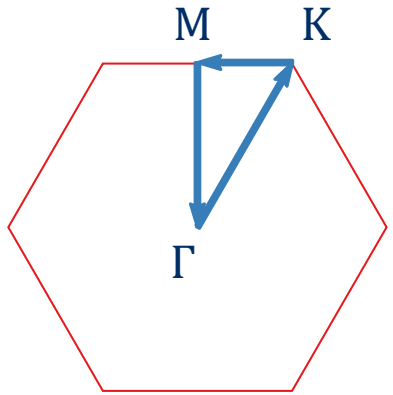


Transition Metal Dichalcogenides

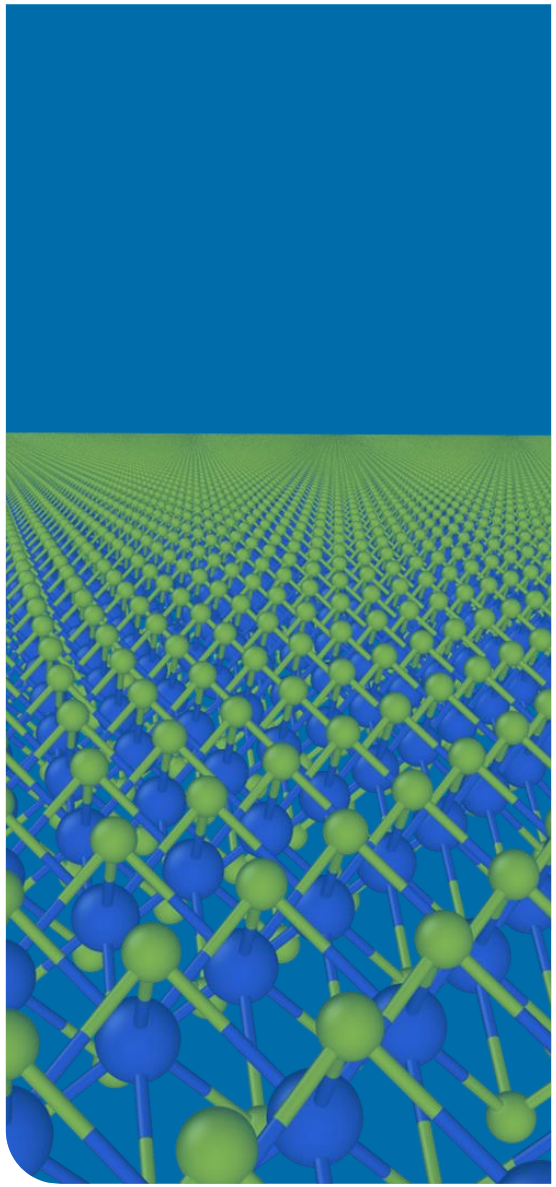


DFT





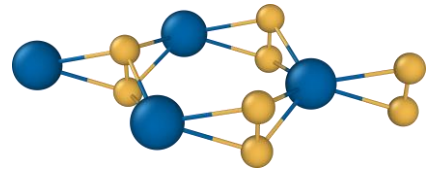
$$\hat{H}_{\mathbf{k}\cdot\mathbf{p}} = f_1 \hat{\sigma} \cdot \mathbf{q} + f_2 \hat{\sigma}_z$$



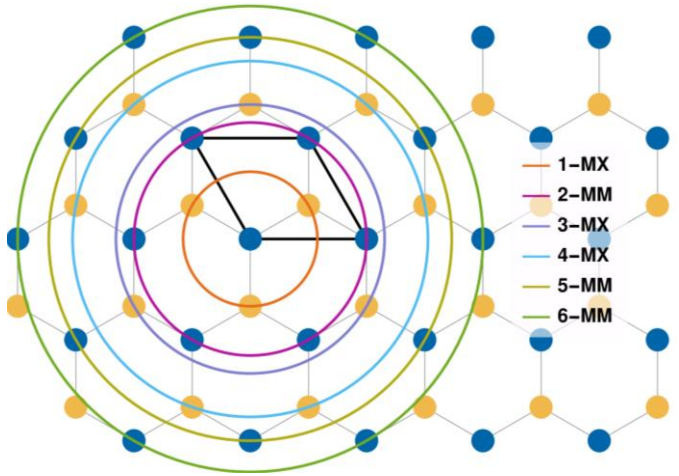
Tight-binding

orbitals - hoppings

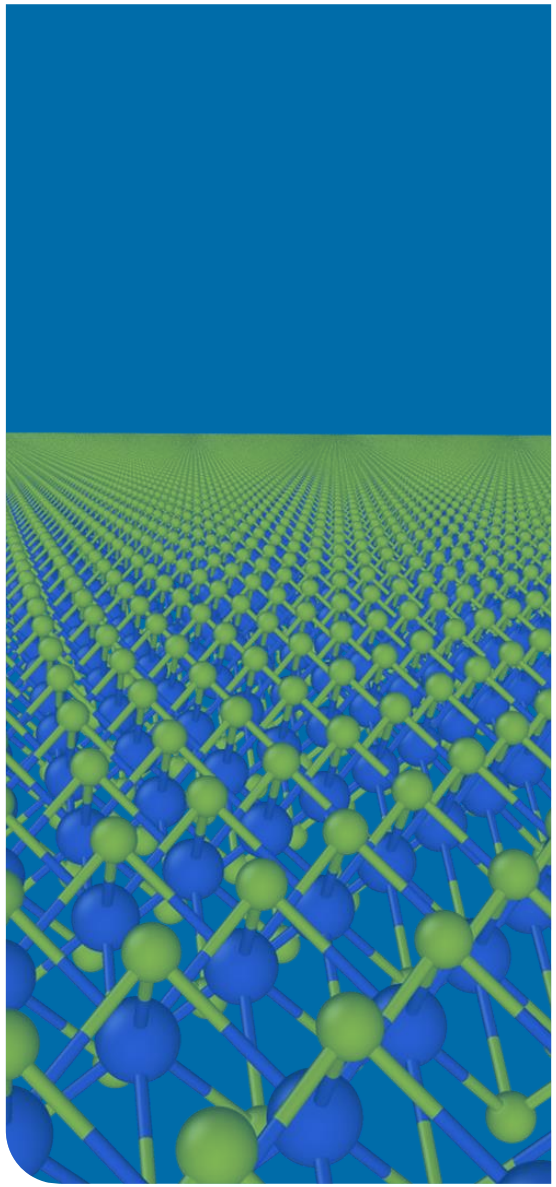
$$\hat{H}_{TB} = \sum_{i,\mu\nu} \varepsilon_{\mu,\nu} \hat{c}^{\dagger}_{i,\mu} \hat{c}_{i,\nu} + \sum_{ij,\mu\nu} \left(t_{ij,\mu\nu} \hat{c}^{\dagger}_{i,\mu} \hat{c}_{j,\nu} + \text{h.c.} \right)$$ [*]



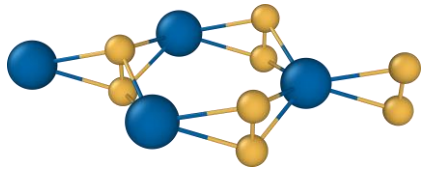
$$\left(d_{z^2}, d_{xz}, d_{yz}, d_{x^2-y^2}, d_{xy}\right),$$
$$\left(p^t_x, p^t_y, p^t_z\right),$$
$$\left(p^b_x, p^b_y, p^b_z\right),$$

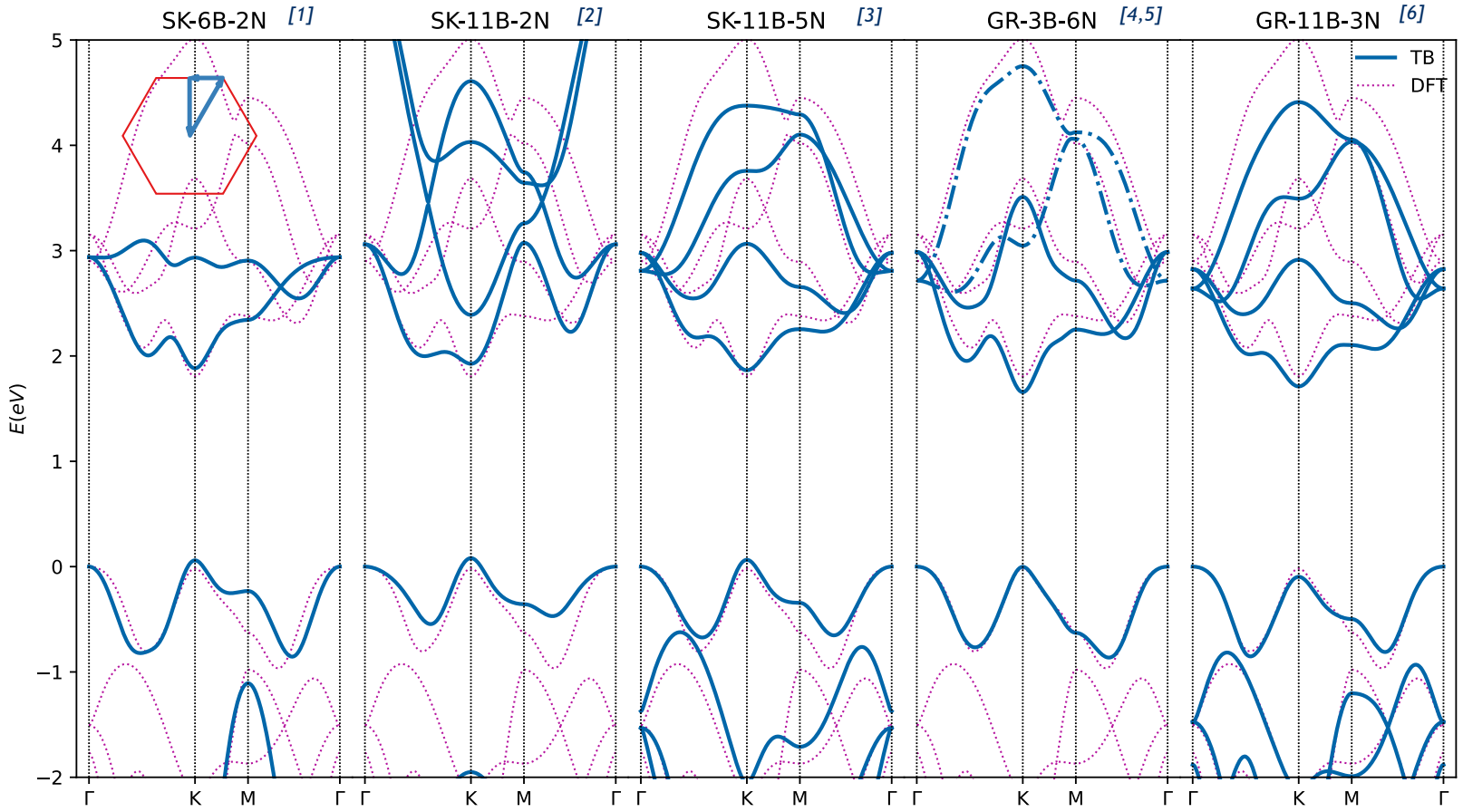


[*] H. Rostami, R. Roldan, E. Cappelluti, R. Asgari, & F. Guinea, Phys. Rev. B 92, 195402 (2015)

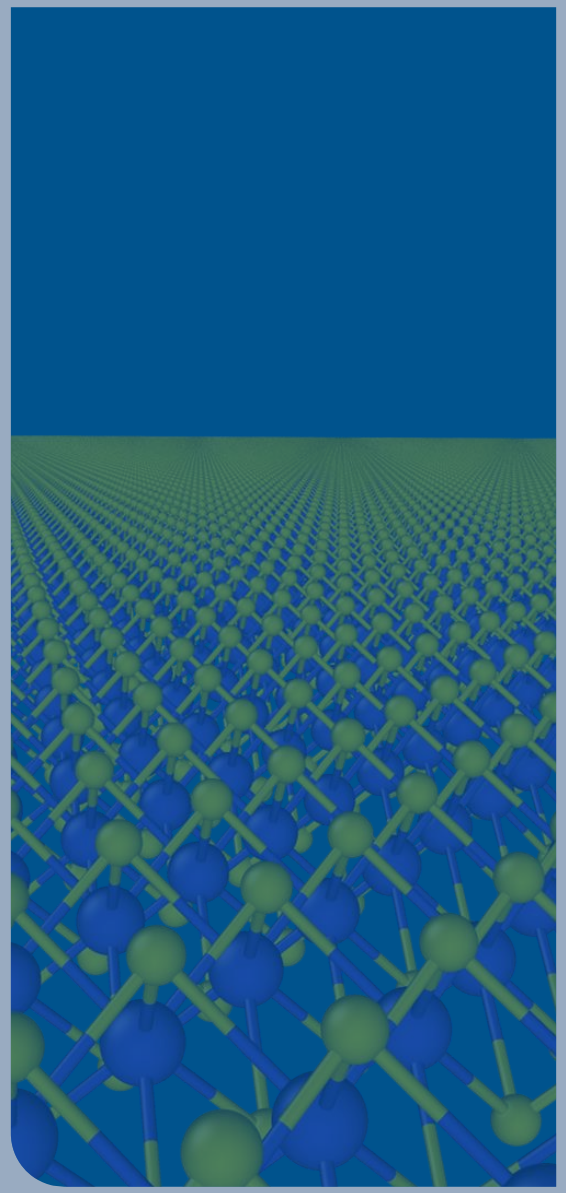


Band structures
original

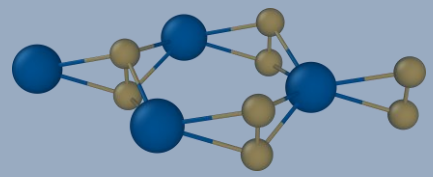


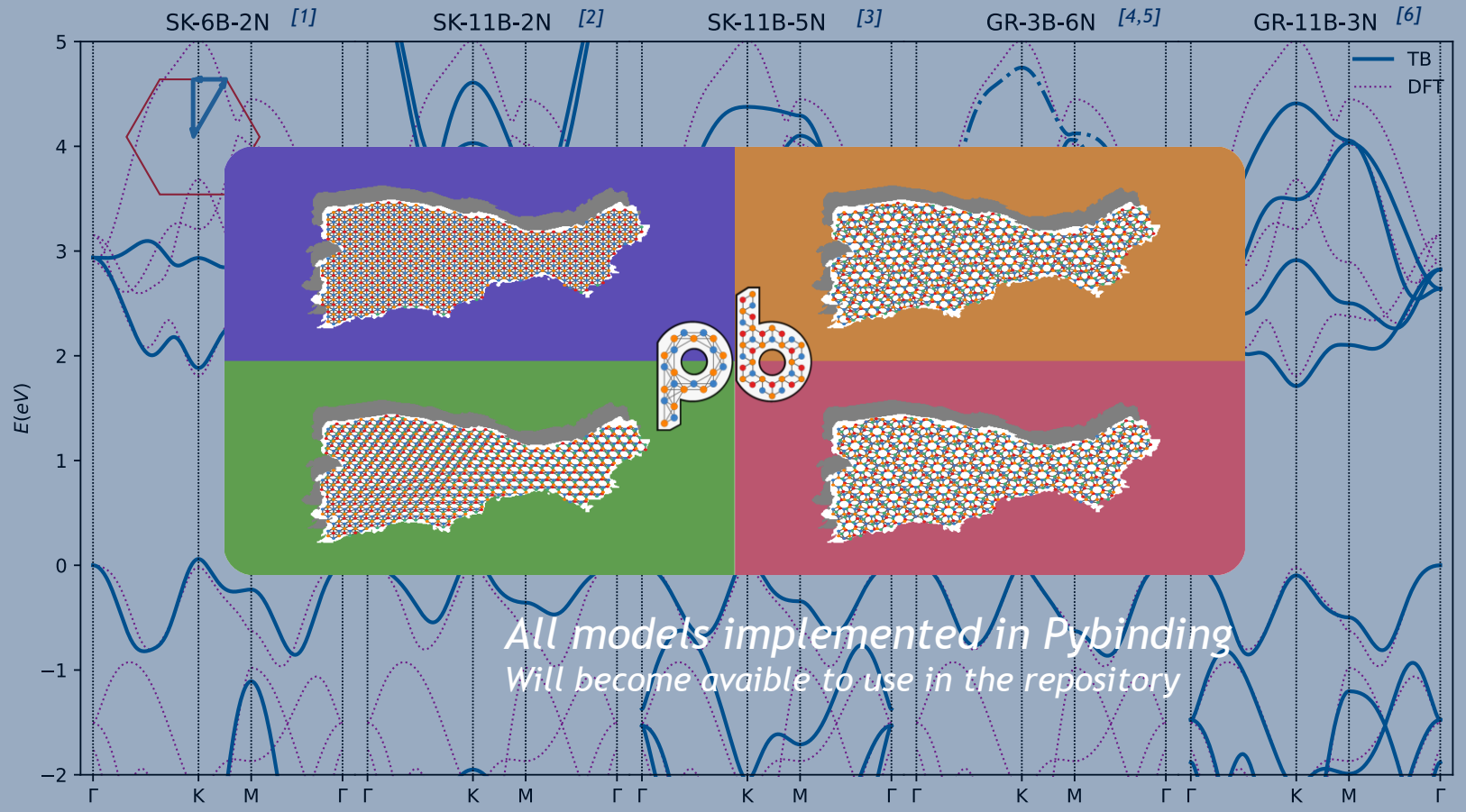


[1] H. Rostami, R. Roldan, E. Cappelluti, R. Asgari, F. Guinea, Phys. Rev. B 92, 195402 (2015)
[2] E. Cappelluti, R. Roldan, J. A. Silva-Guillen, P. Ordejon, F. Guinea, Phys. Rev. B 88, 075409 (2013)
[3] A. C. Dias, F. Qu, D. L. Azevedo, J. Fu, Phys. Rev. B 98, 075202 (2018)
[4] G.-B. Liu, W.-Y. Shan, Y. Yao, W. Yao, and D. Xiao, Phys. Rev. B 88, 085433 (2013)
[5] F. Wu, F. Qu, and A. H. MacDonald, Phys. Rev. B 91, 075310 (2015)
[6] S. Fang, R. Kuate Defo, S. N. Shirodkar, S. Lieu, G. A. Tritsaris, and E. Kaxiras, Phys. Rev. B 92, 205108 (2015)



Band structures
original





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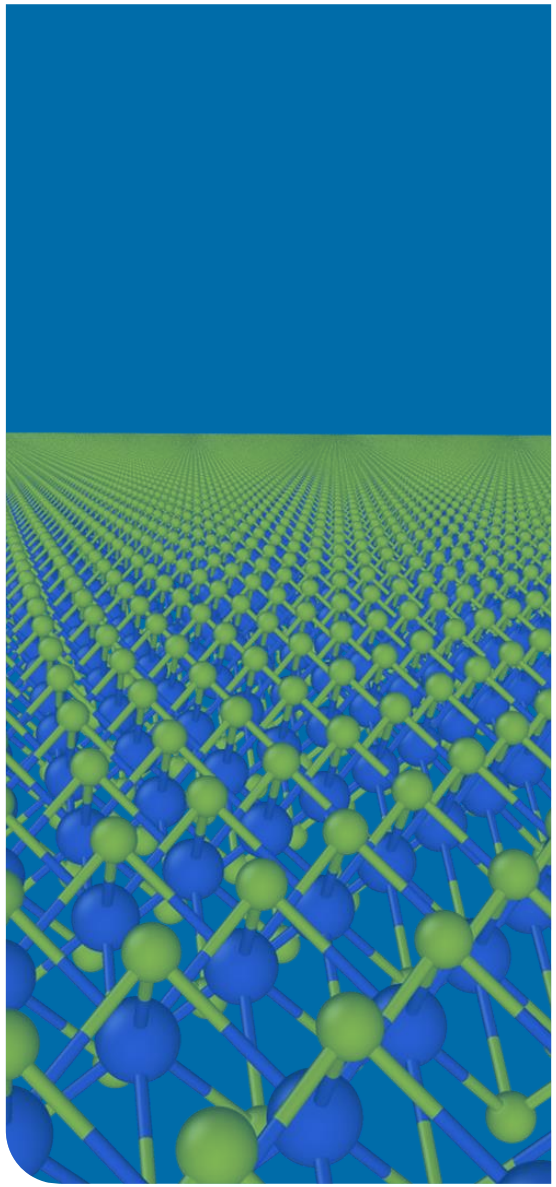
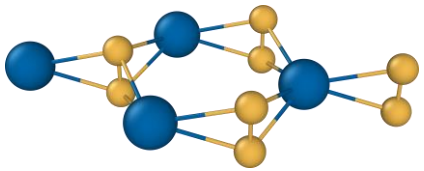
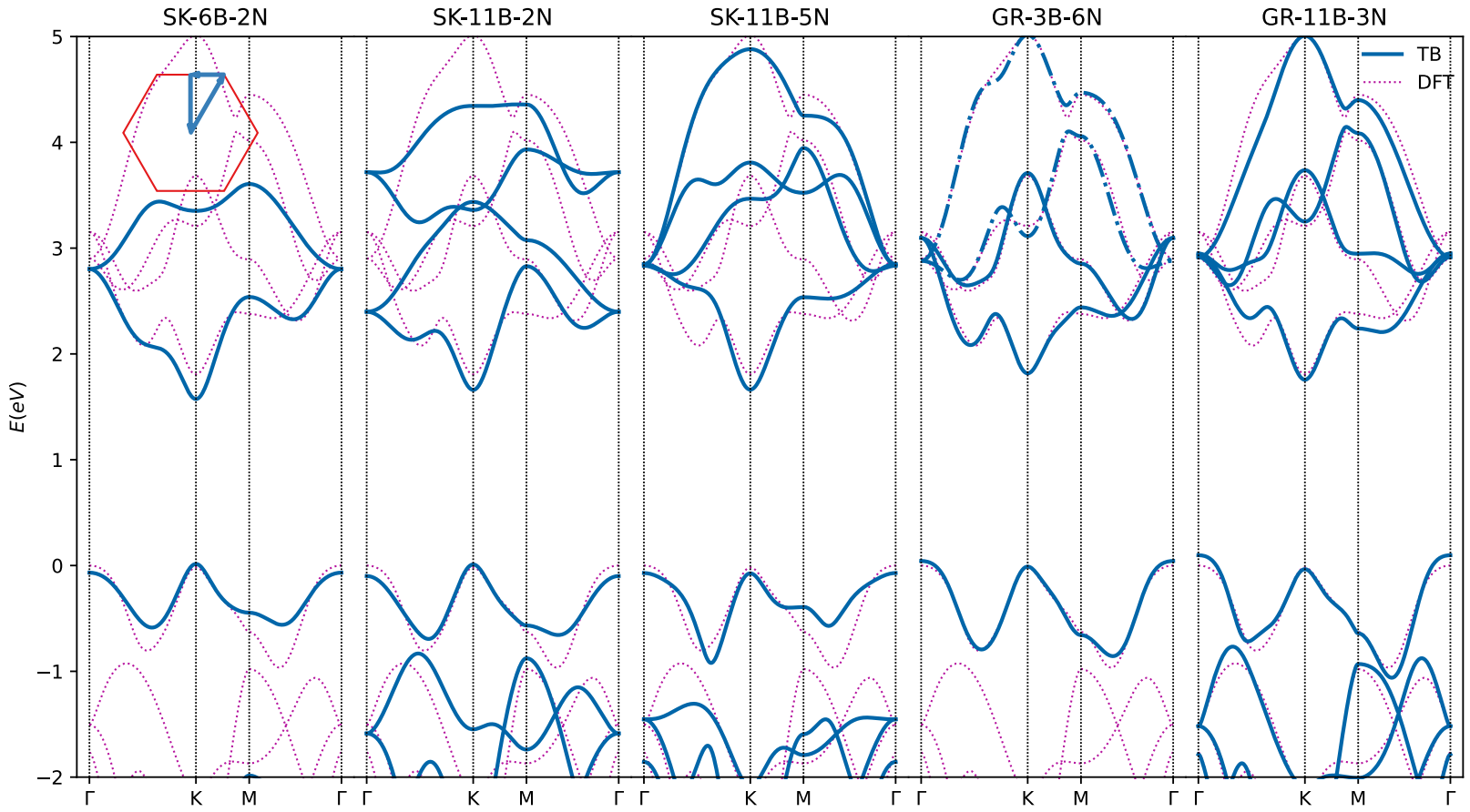
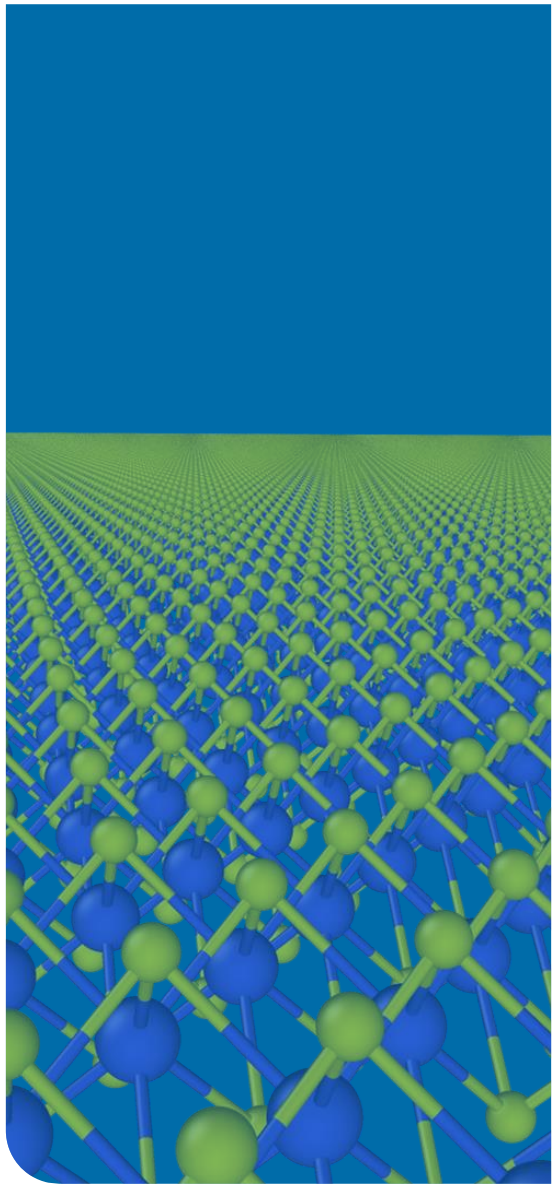


Band structures

my fit

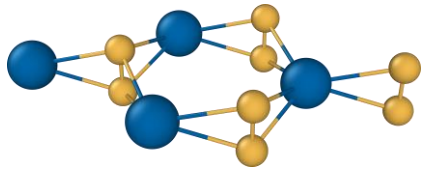


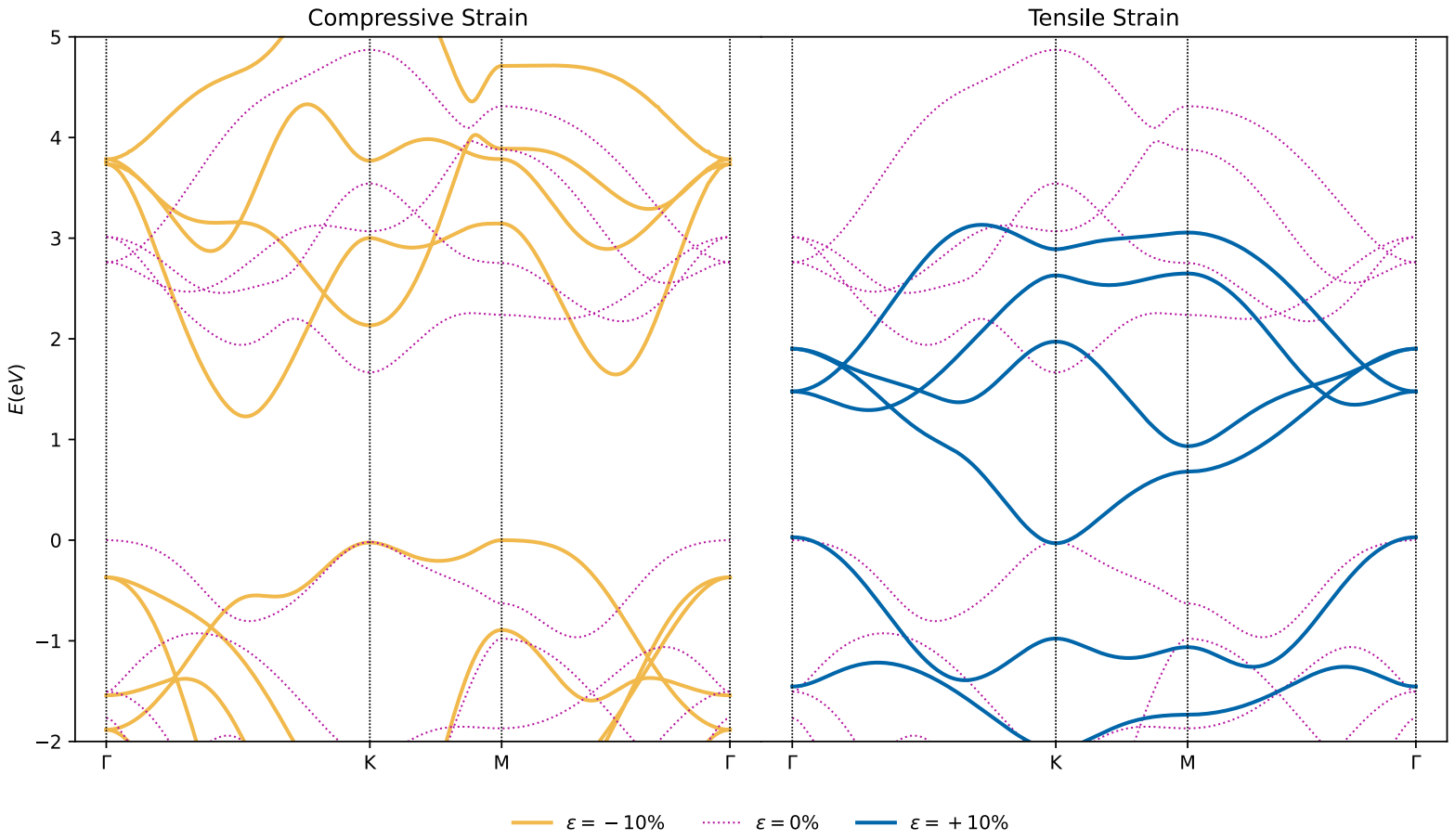


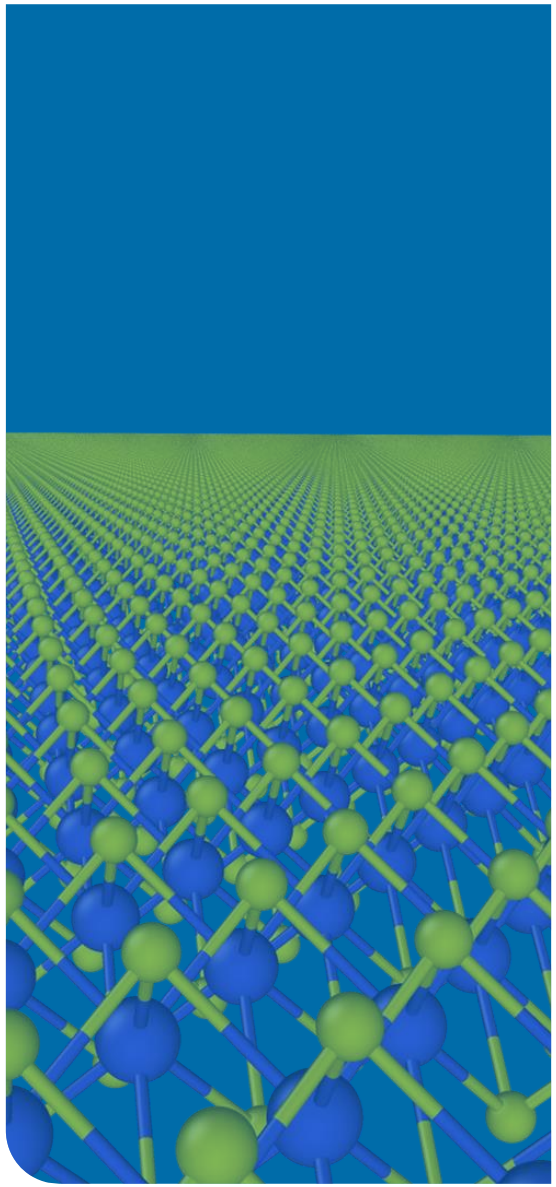


Adding strain

DFT

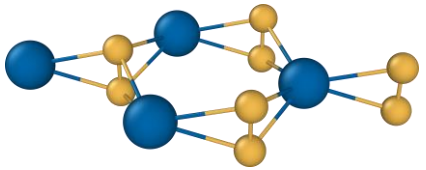


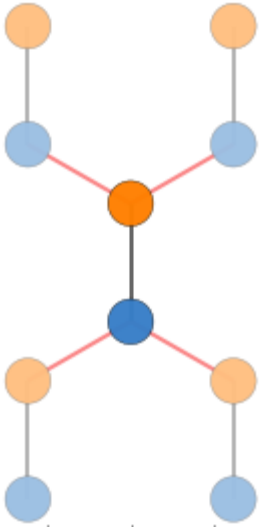




Adding strain

graphene



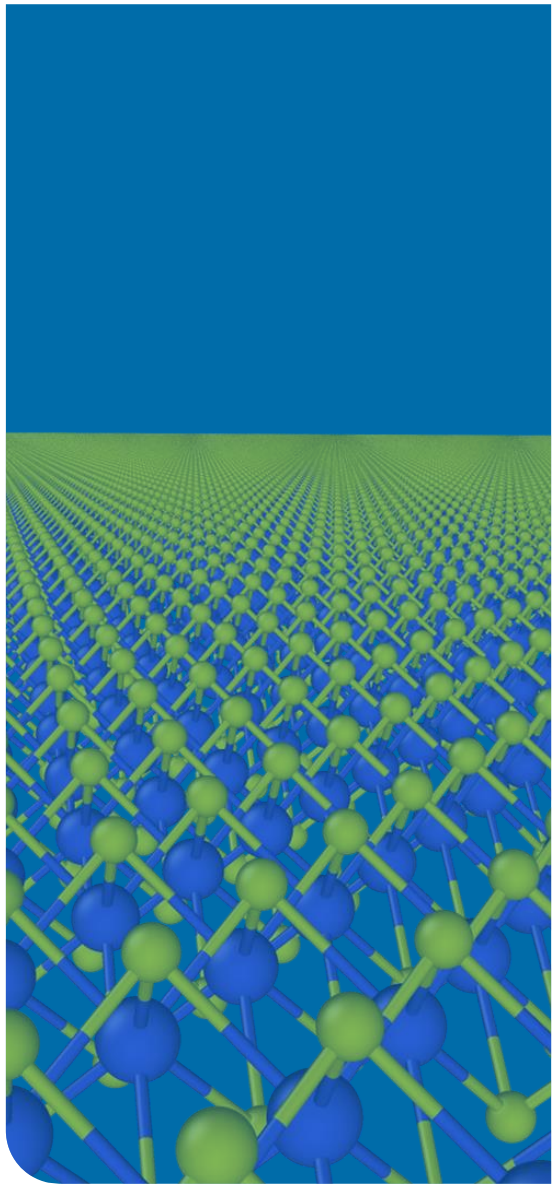


$$\begin{cases} A_x = \varepsilon_{xx} - \varepsilon_{yy} \\ A_y = -2\varepsilon_{xy} \end{cases}$$

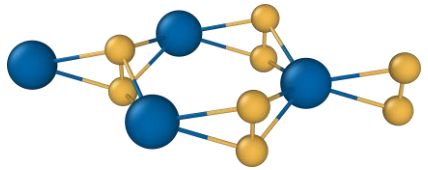
$$B = \nabla \times A$$

Pseudo Magnetic Field

$$\hat{H}_{\mathbf{kp}} = \hbar v_F \hat{\sigma} \cdot \mathbf{q} + \beta \mathbf{A} \cdot \hat{\sigma}$$



Adding strain
TMD

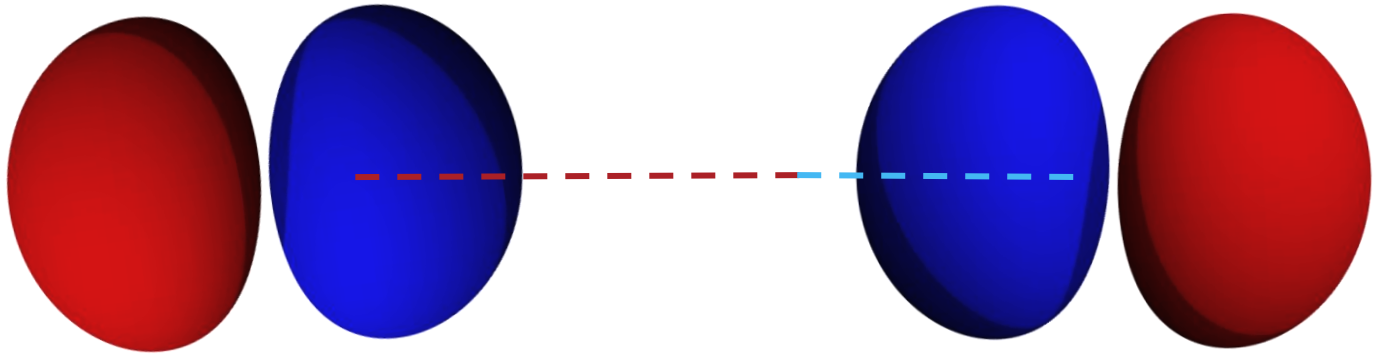


$$\hat{H}_{TB} = \sum_{i,\mu\nu} \varepsilon_{\mu,\nu} \hat{c}^{\dagger}_{i,\mu} \hat{c}_{i,\nu} + \sum_{ij,\mu\nu} \left(t_{ij,\mu\nu} \hat{c}^{\dagger}_{i,\mu} \hat{c}_{j,\nu} + \text{h.c.} \right)$$

$$t_{ij,\mu\nu}(\mathbf{r}_{ij}) = t_{ij,\mu\nu}\left(\mathbf{r}^0_{ij}\right)\left(1 - \Lambda_{ij,\mu\nu}\frac{\left|\mathbf{r}_{ij} - \mathbf{r}^0_{ij}\right|}{\left|\mathbf{r}^0_{ij}\right|}\right), \qquad (4)^{[*]}$$

$\sim V_{pp\pi}$ …

Bond resolved electron-phonon coupling



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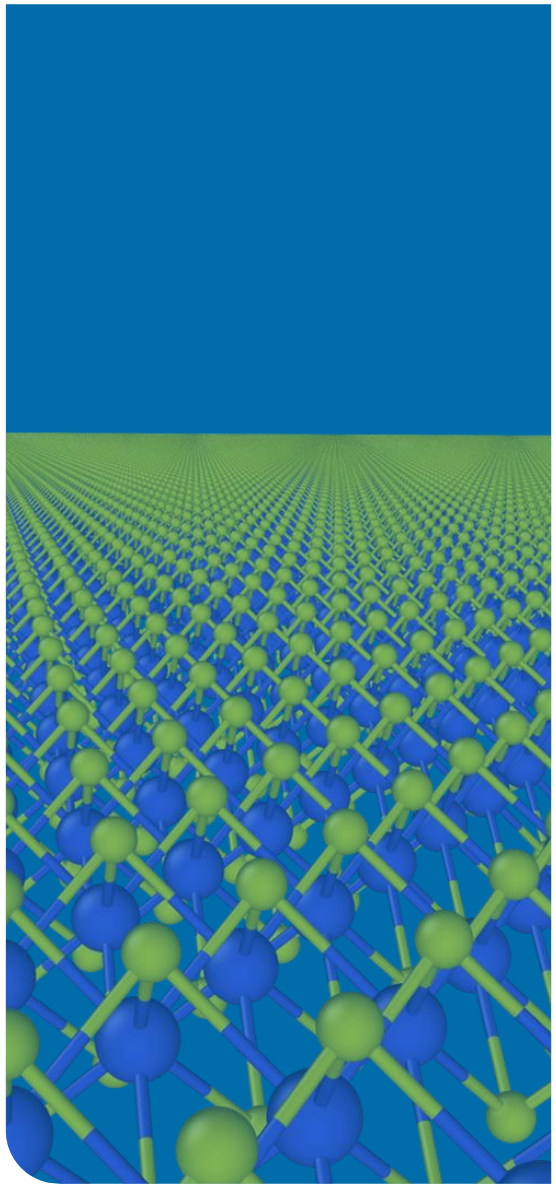
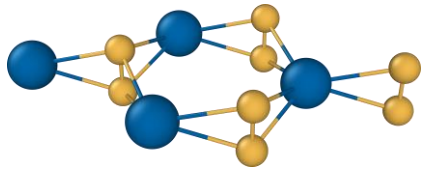
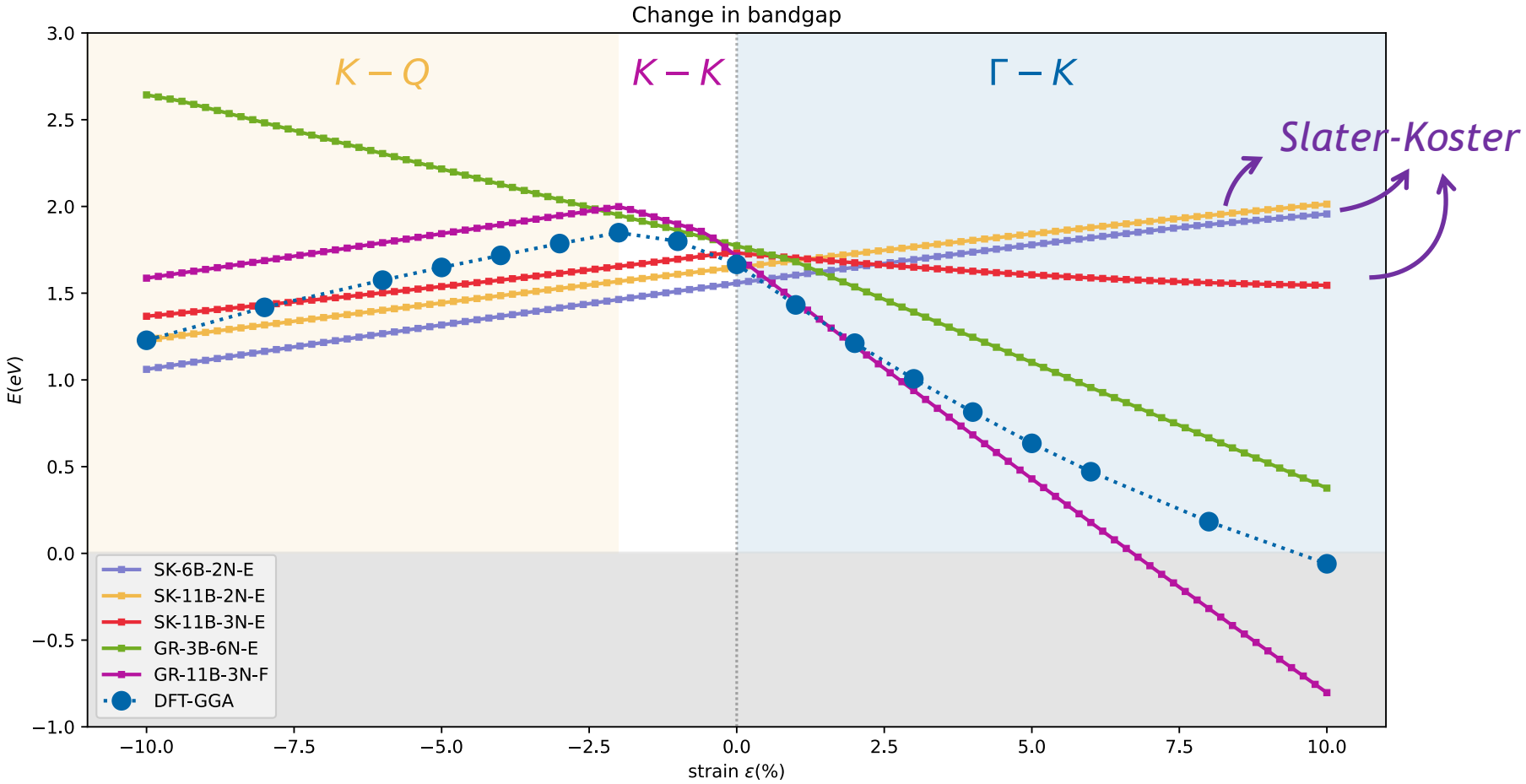
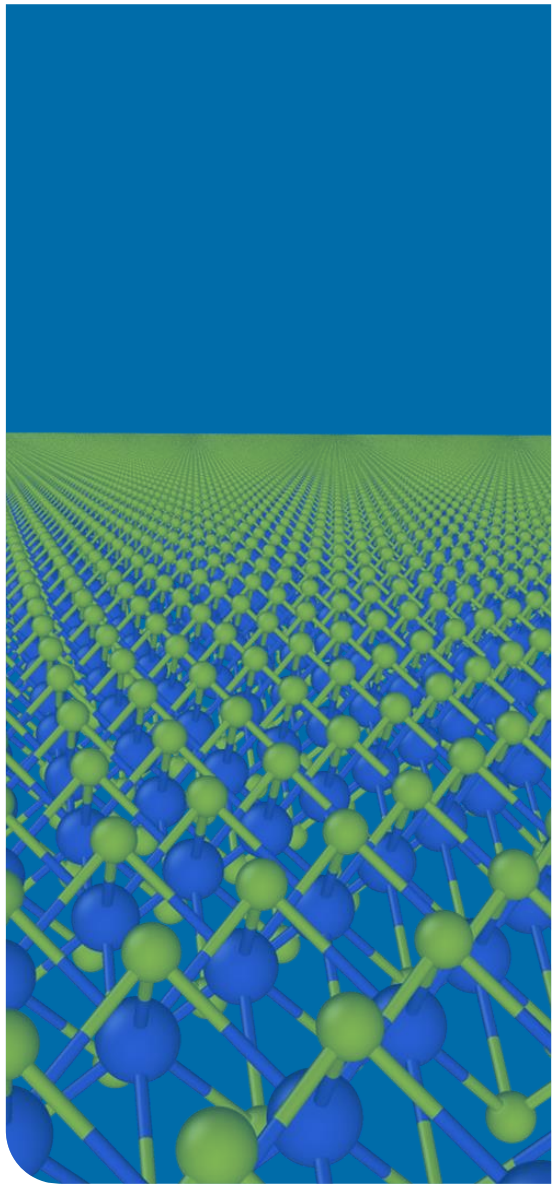


Adding strain

Band gap

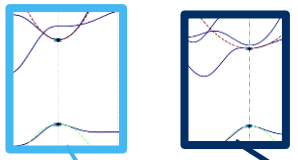


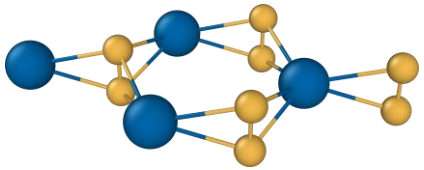




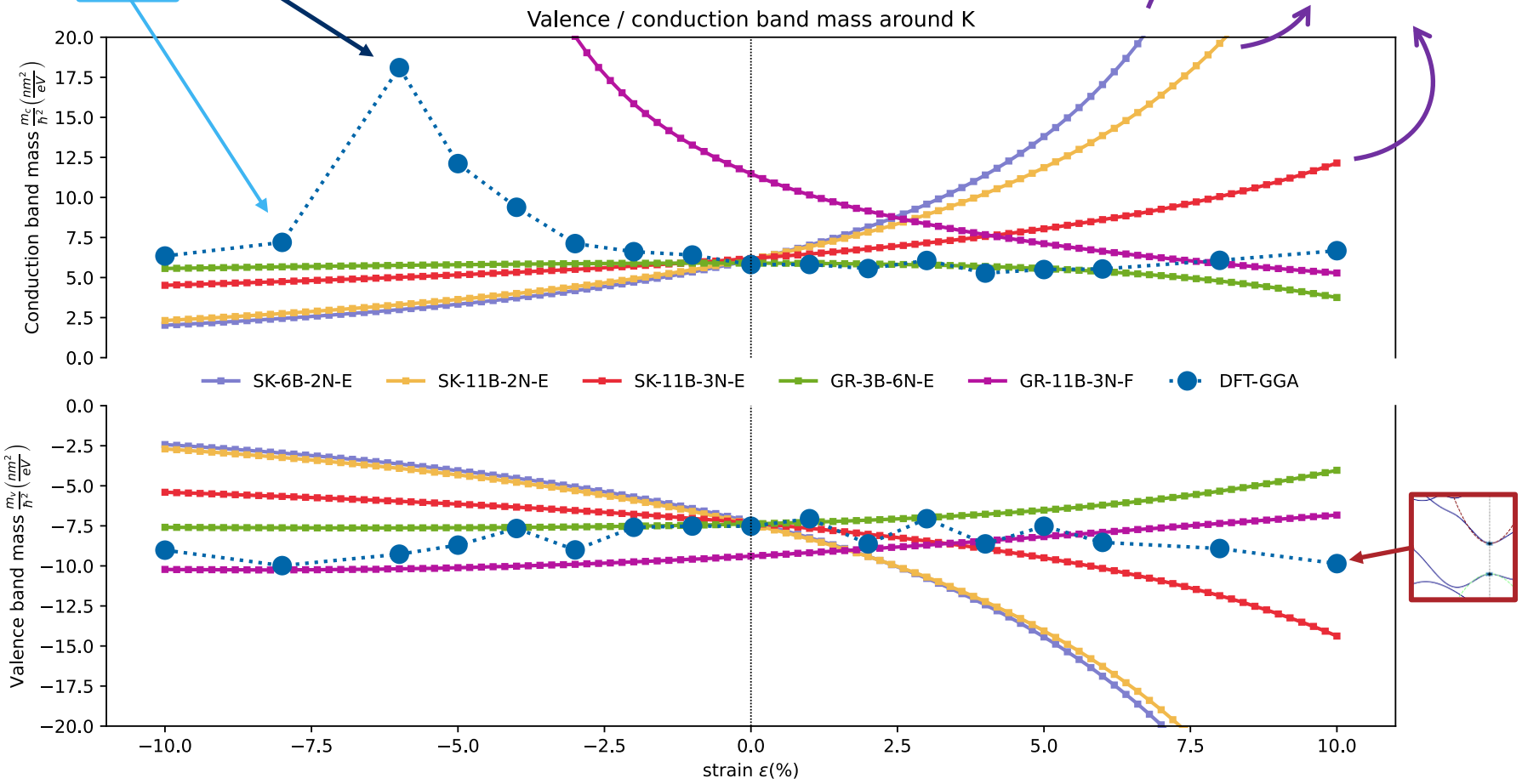
Adding strain

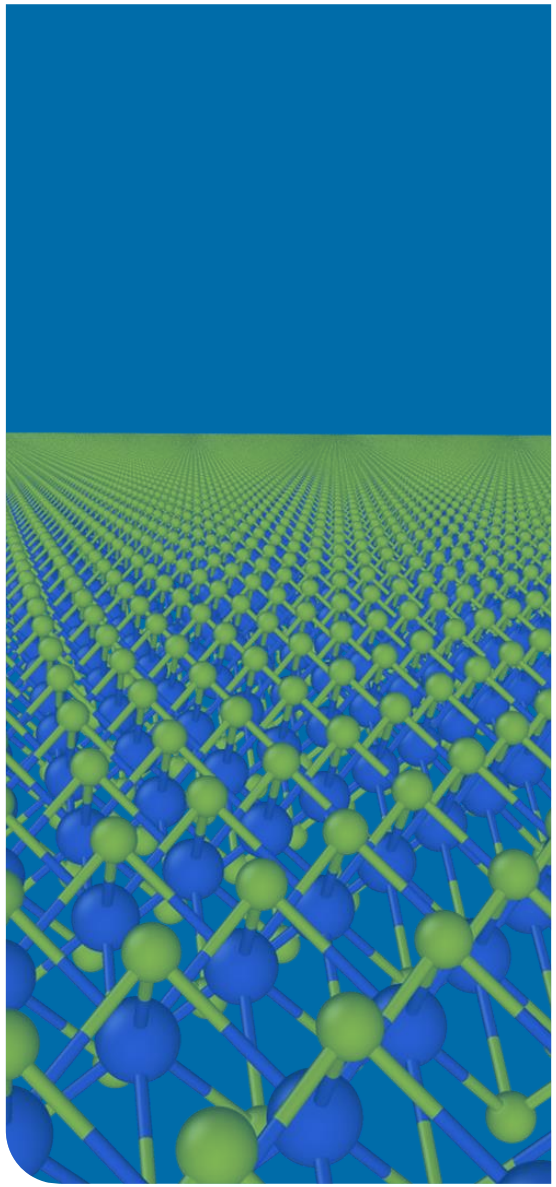
effective mass



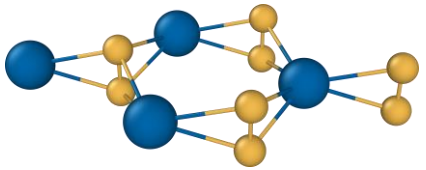


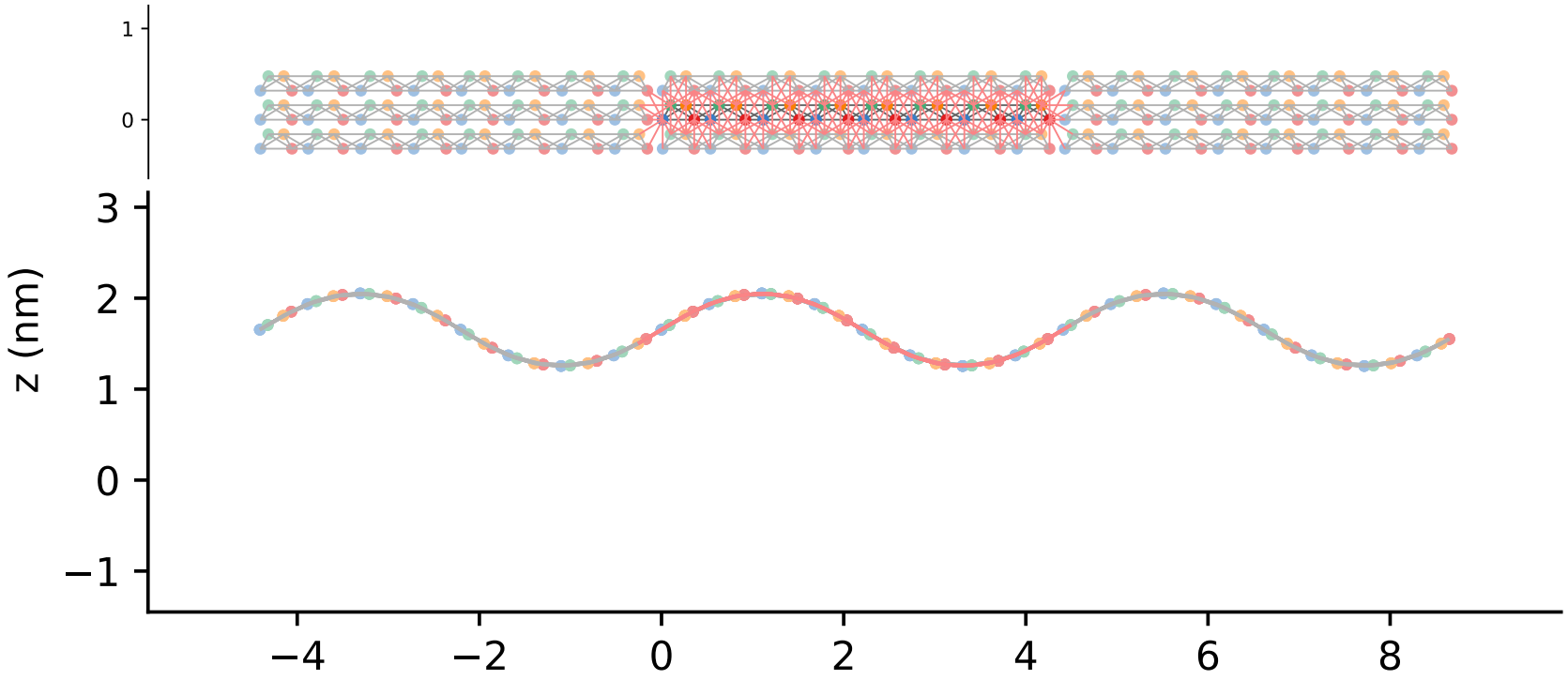
Slater-Koster

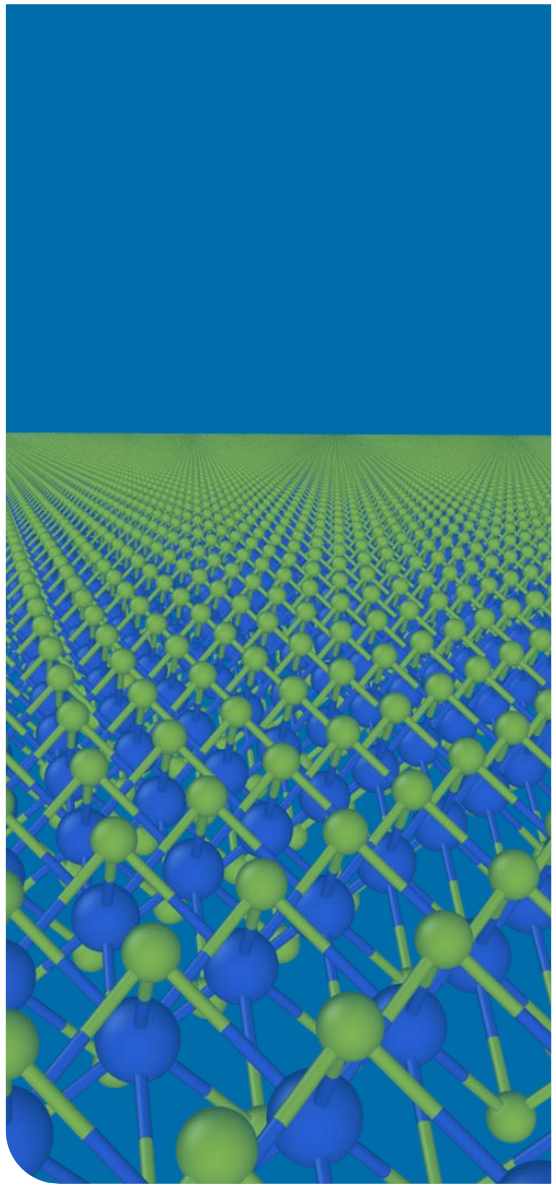




1D sine strain







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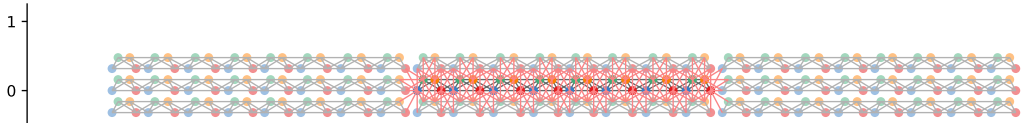
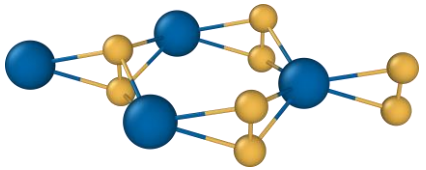
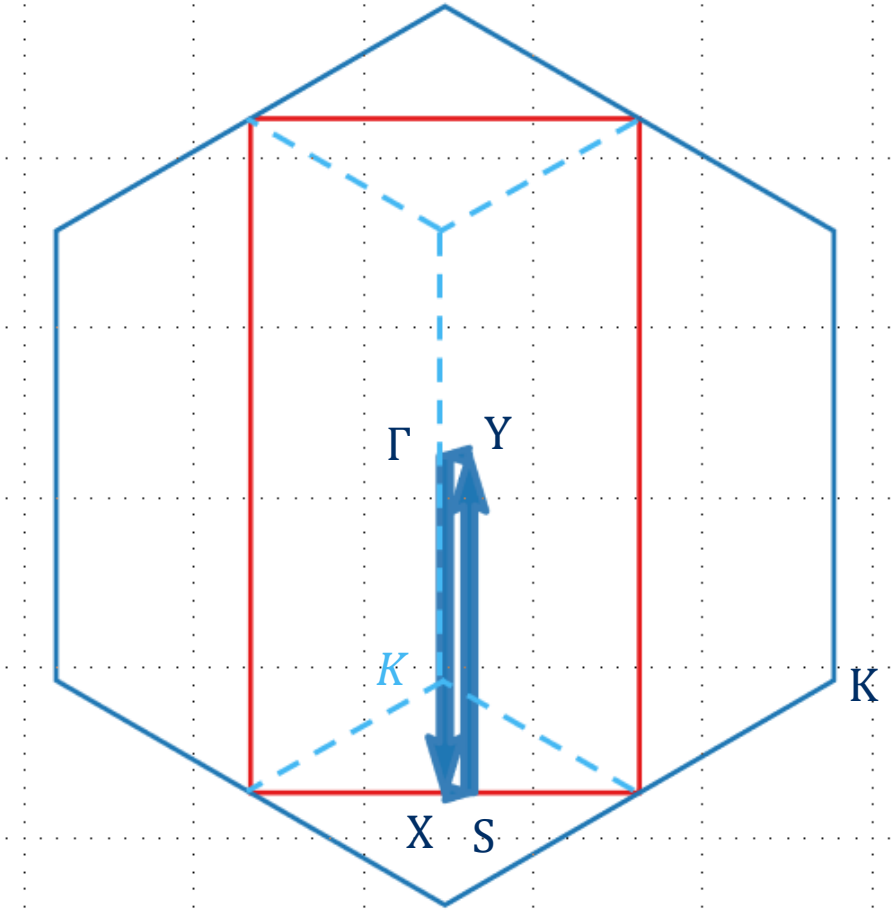
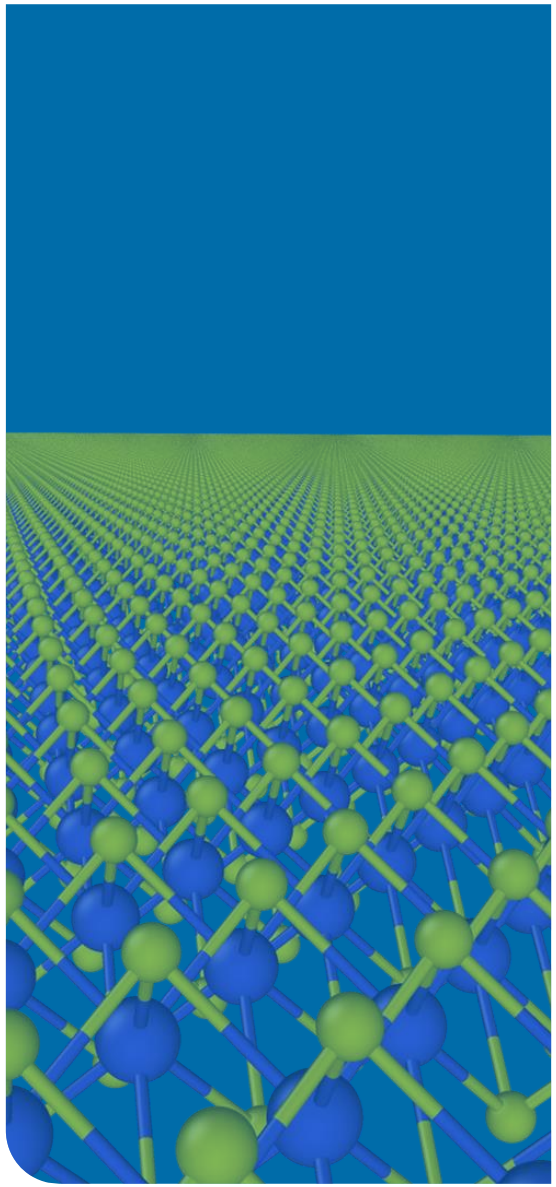


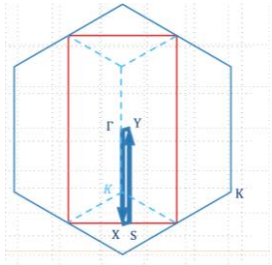




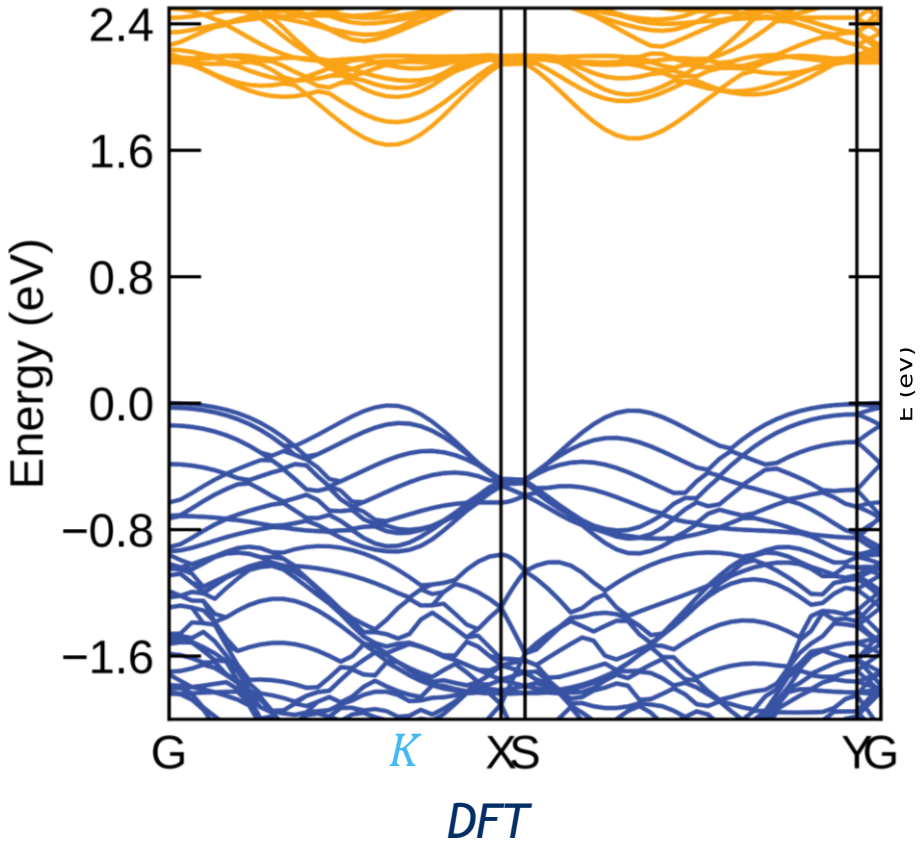


1D sine strain

DFT vs TB



Slater-Koster – 11B-5N



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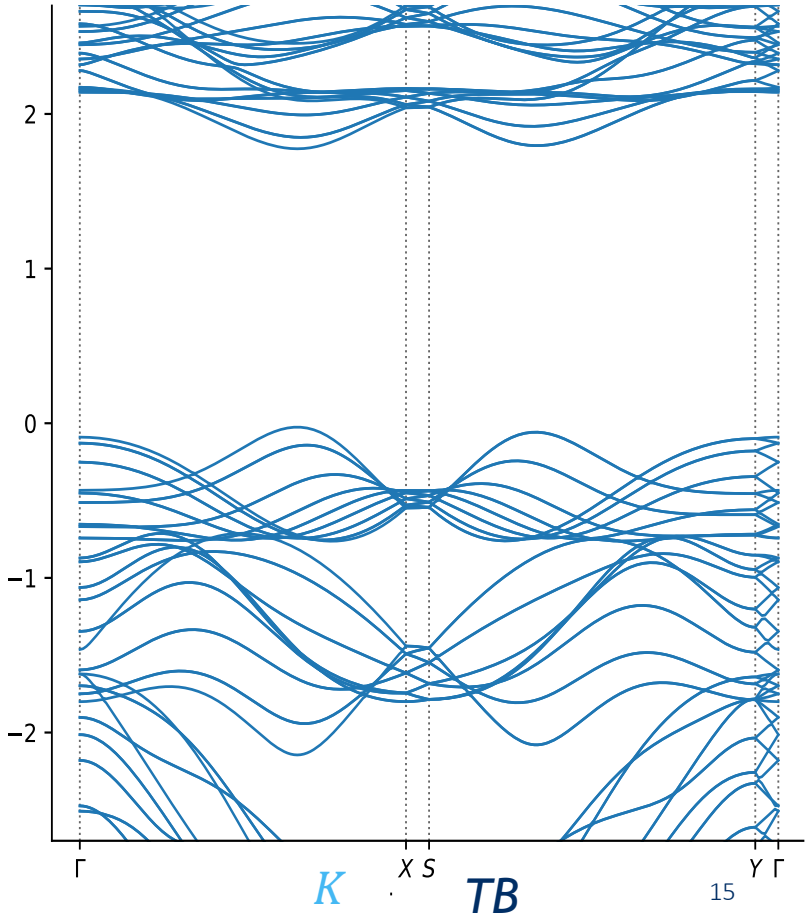
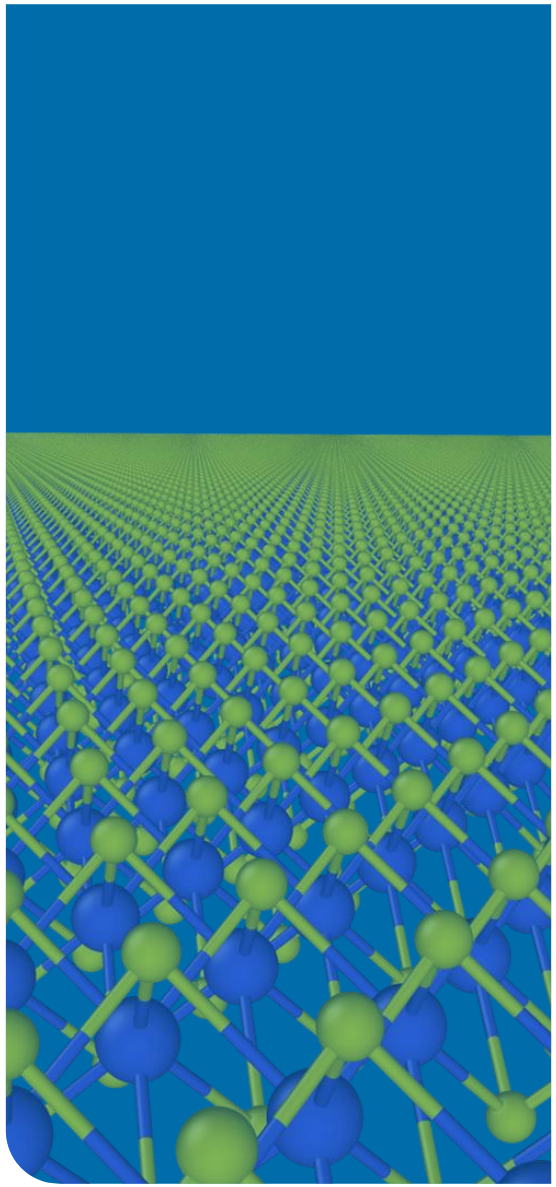
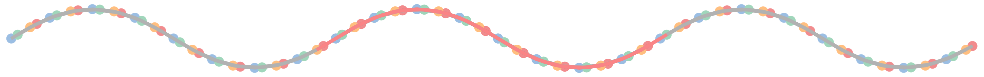


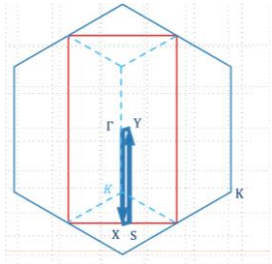
TB



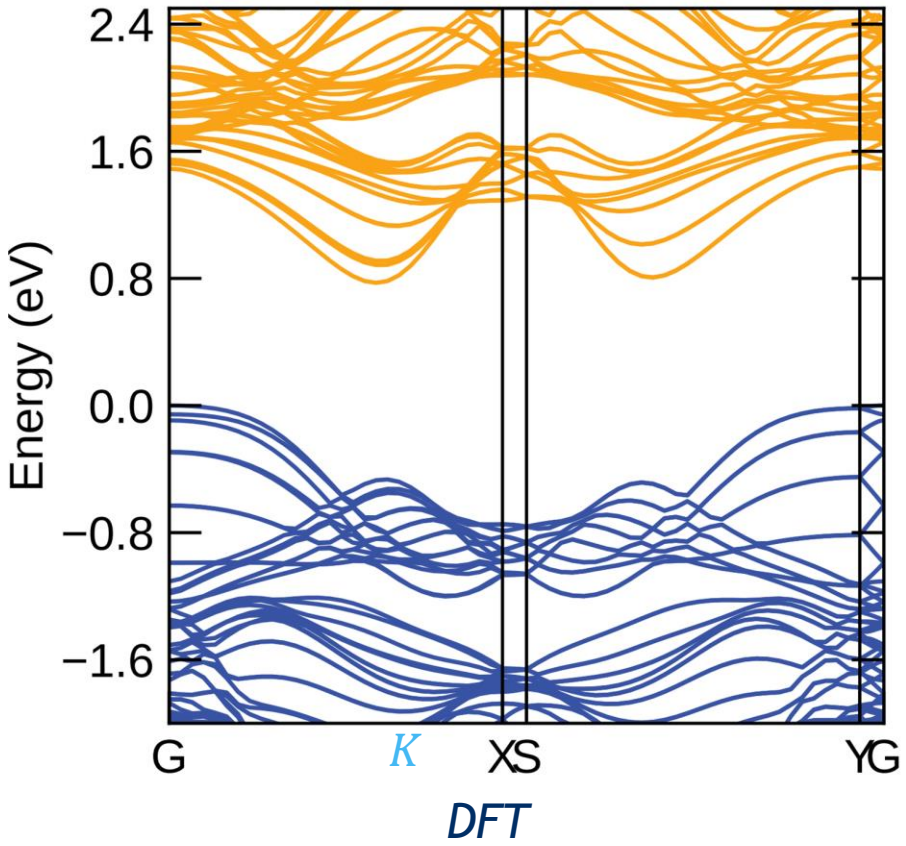
1D sine strain

DFT vs TB

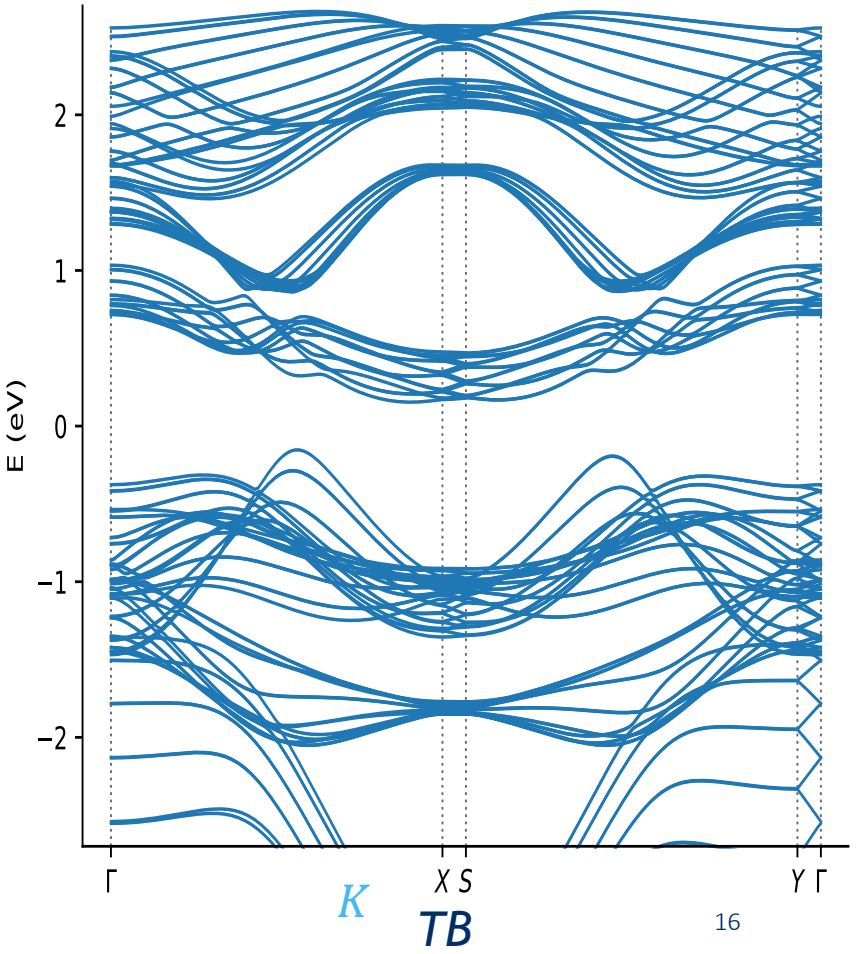




Slater-Koster – 11B-5N

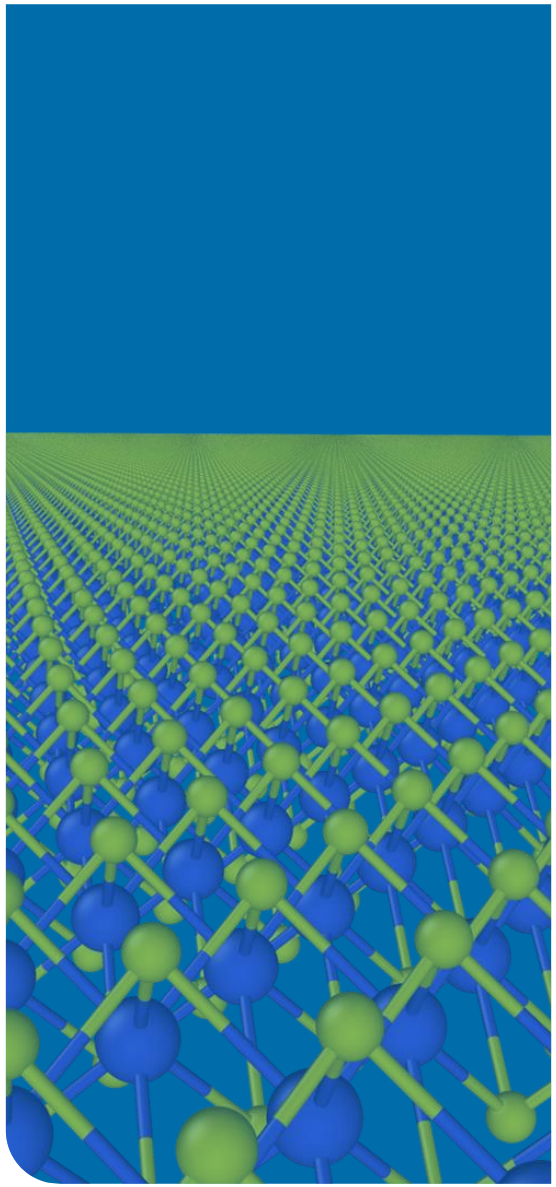


DFT



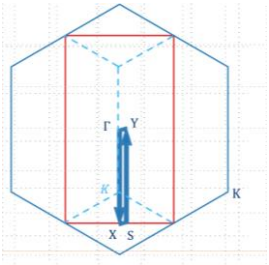
TB

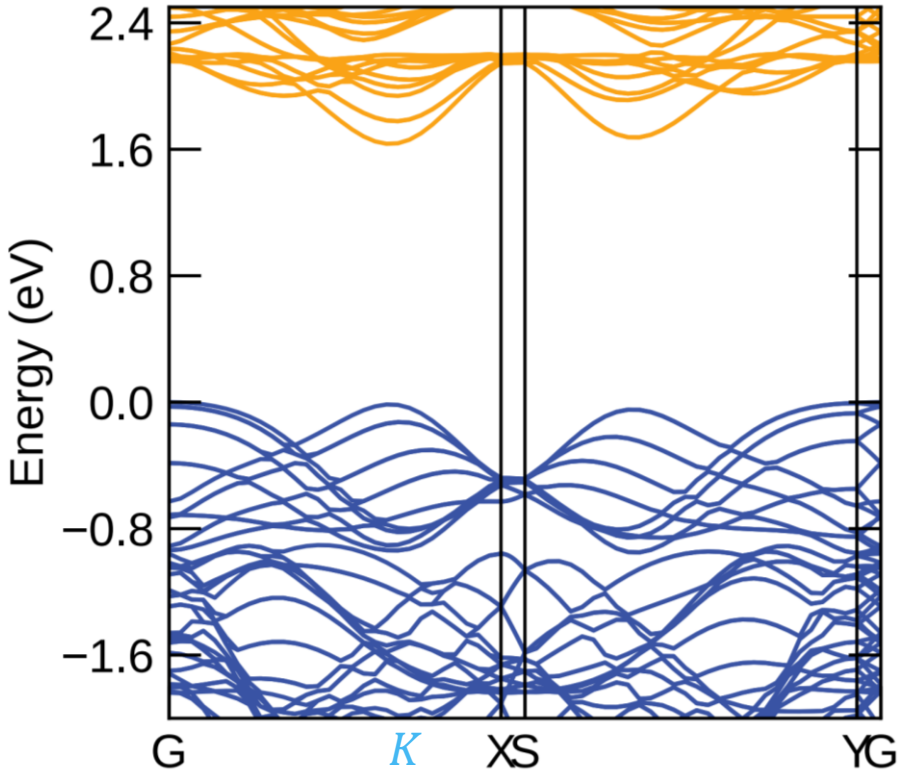
University of Antwerp
I CMT I Condensed Matter Theory



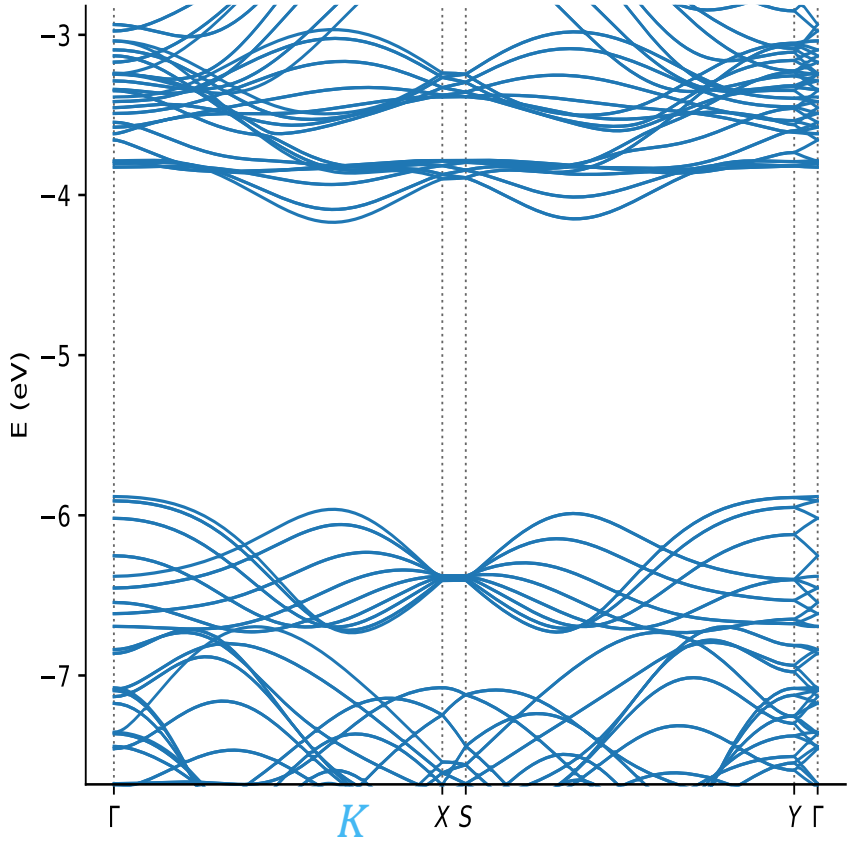
1D sine strain

DFT vs TB

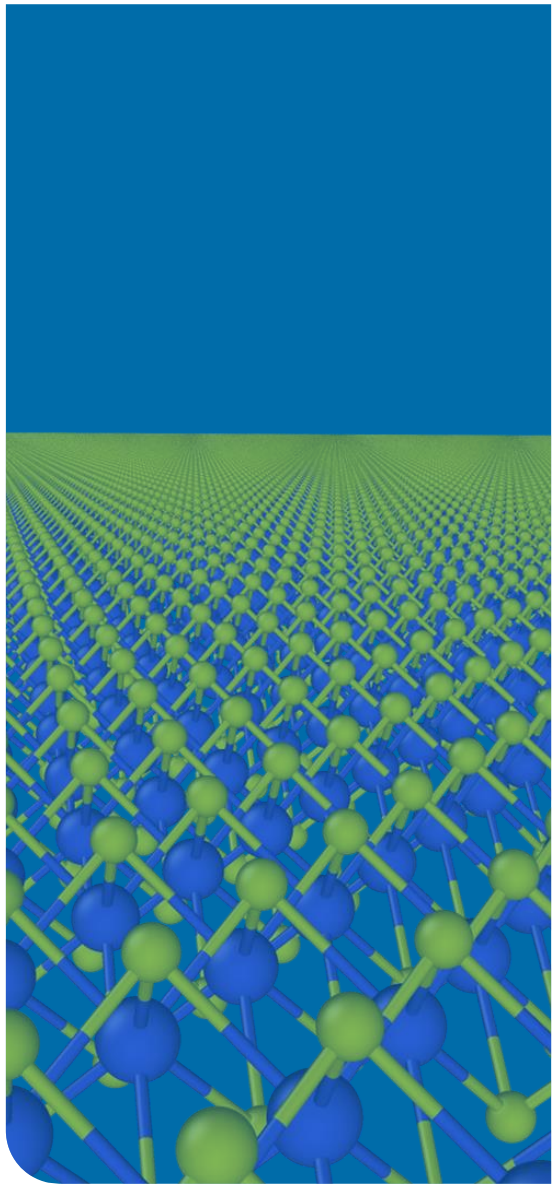




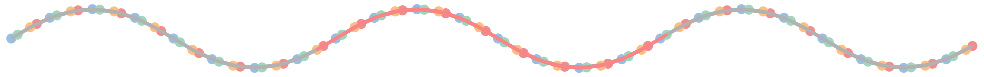
DFT



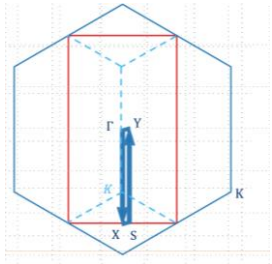
TB

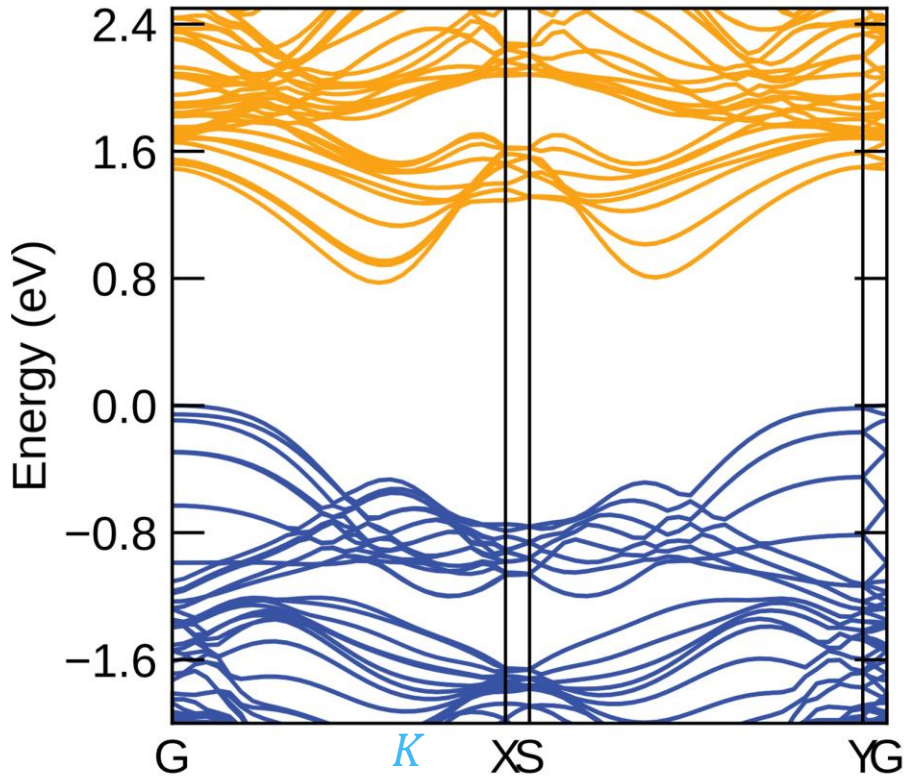


1D sine strain

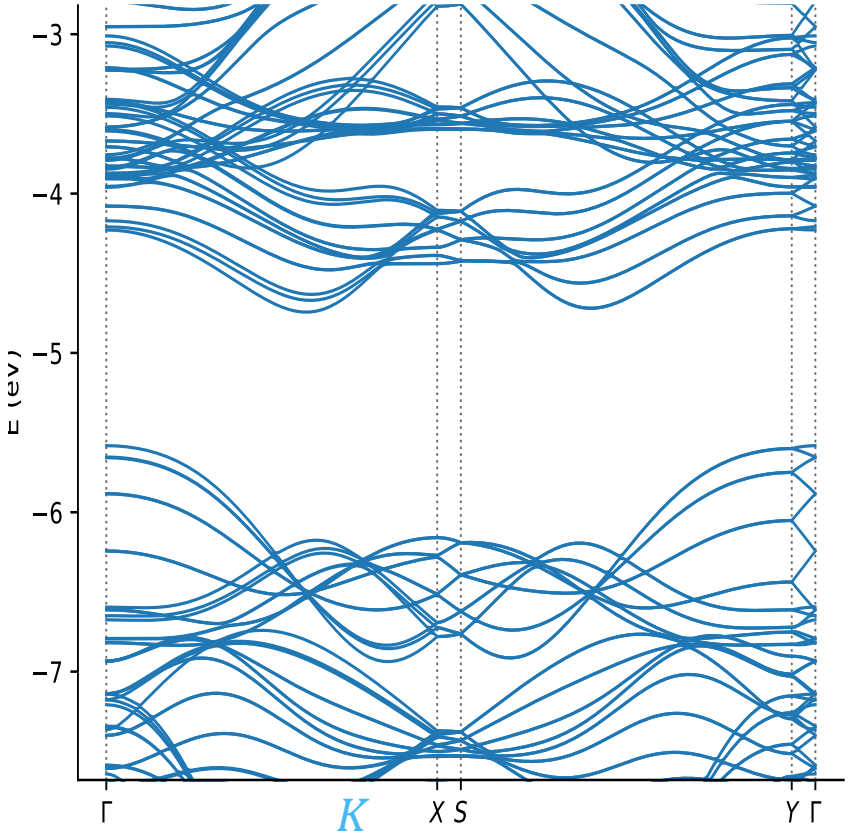


DFT vs TB

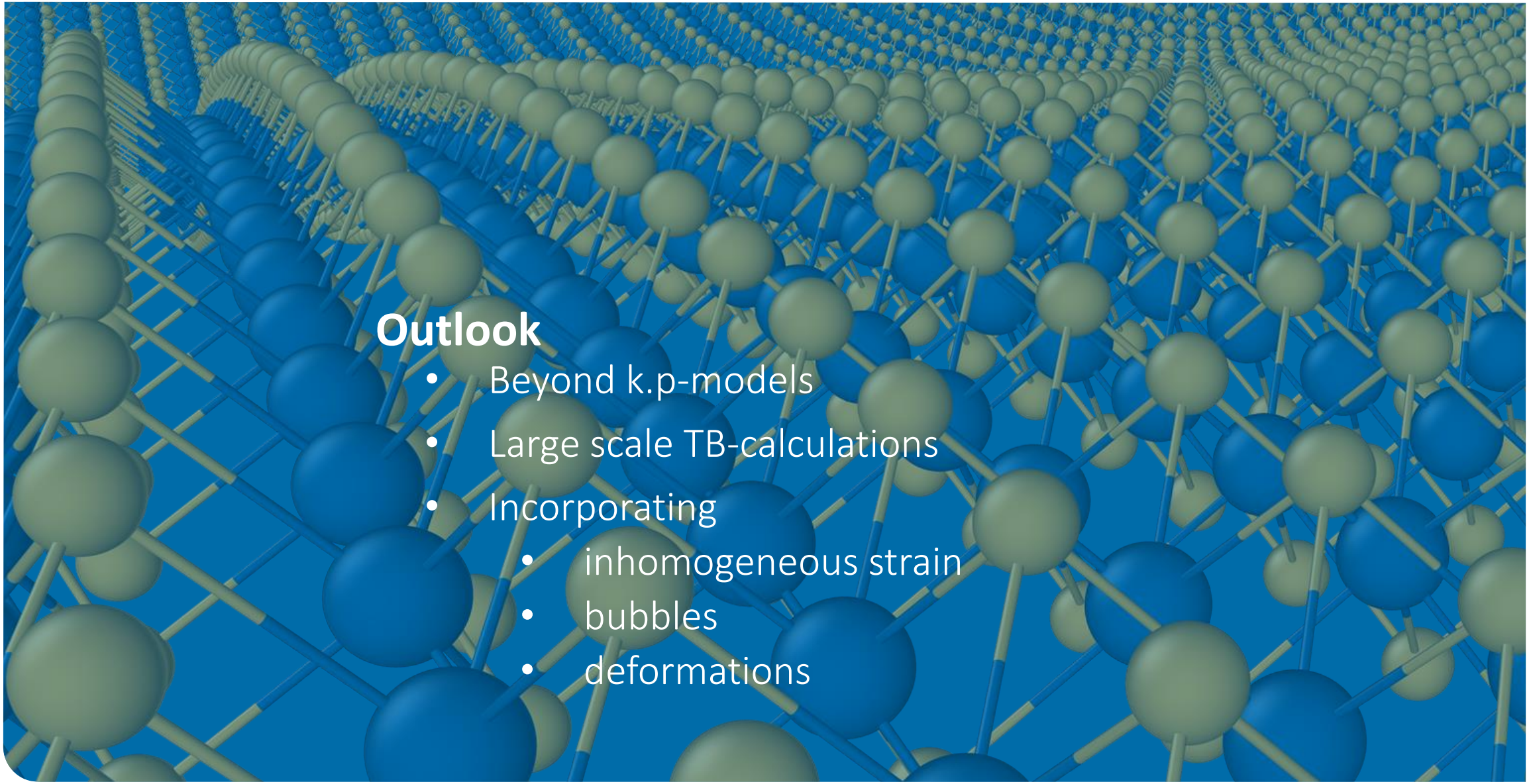




DFT



TB


Outlook
• Beyond k.p-models
• Large scale TB-calculations
• Incorporating
• inhomogeneous strain
• bubbles
• deformations