Piezoelectricity in asymetrically strained bilayer graphene

Matthias Van der Donck

Universiteit Antwerpen

Introduction

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The electric charge that accumulates in certain solid materials in response to applied mechanical stress.

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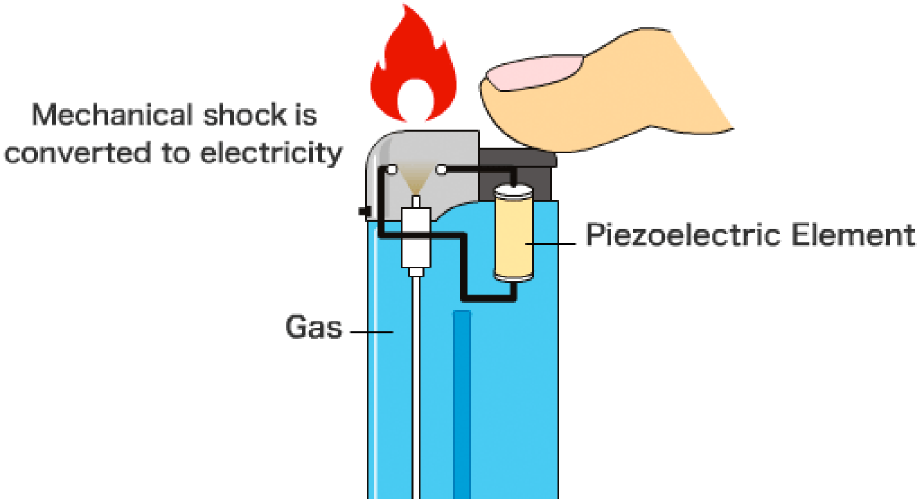

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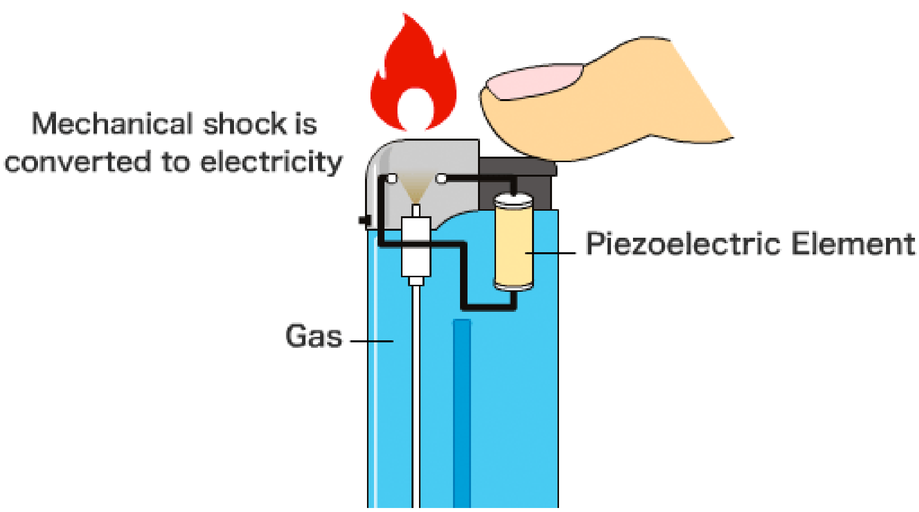

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Pristine

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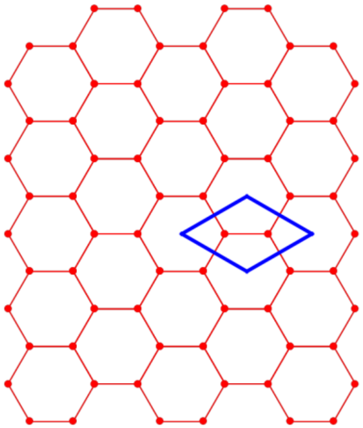

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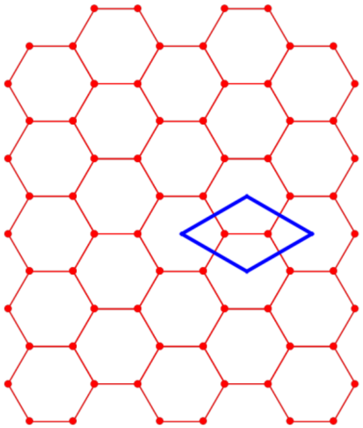

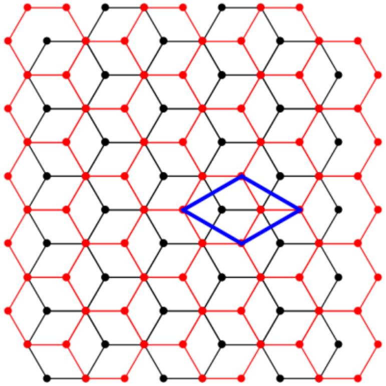

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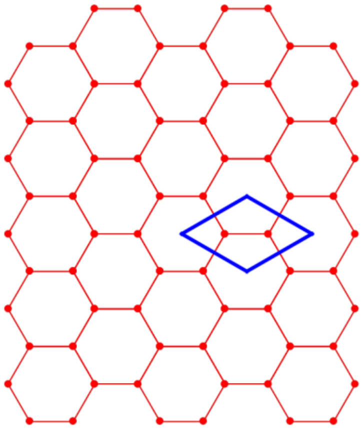

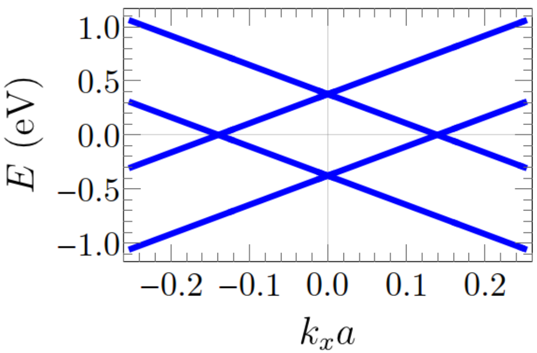

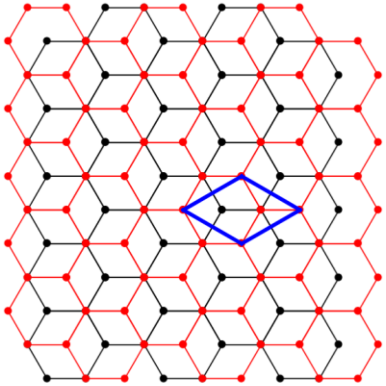

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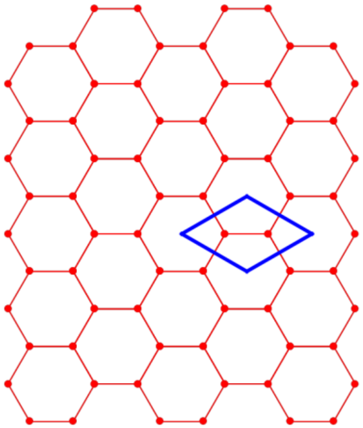

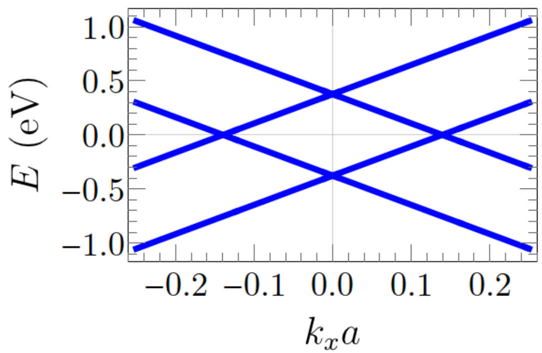

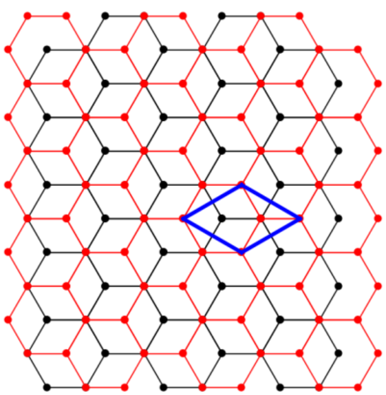

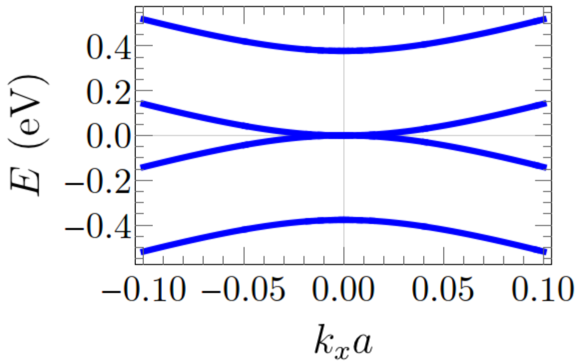

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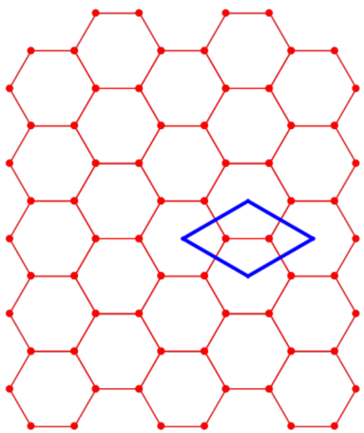

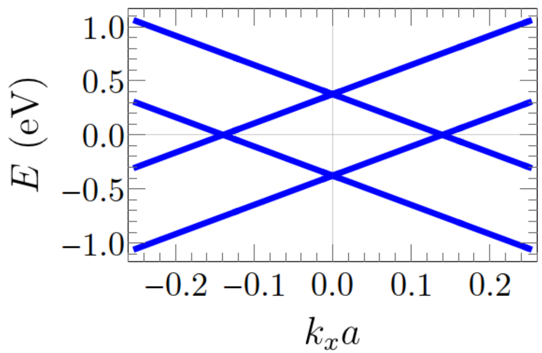

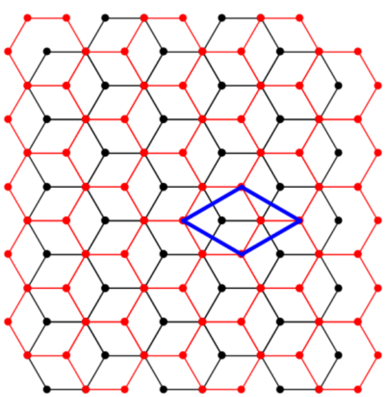

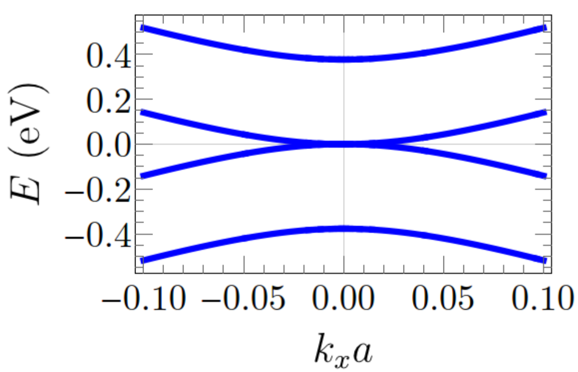

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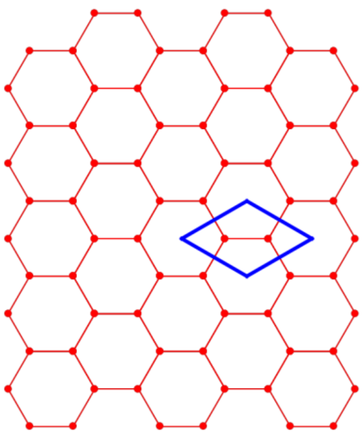

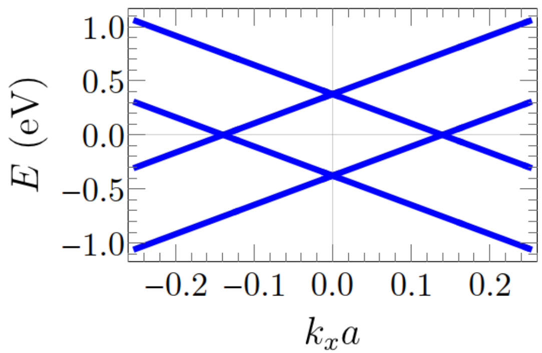

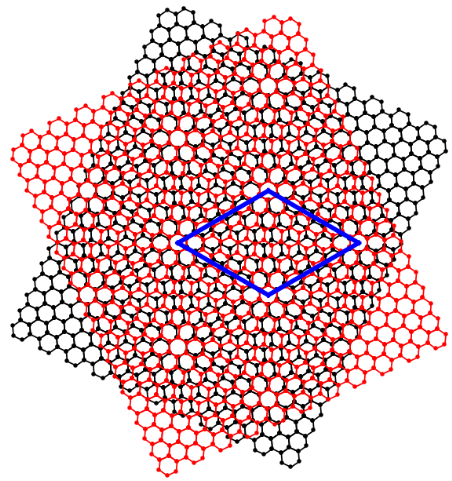

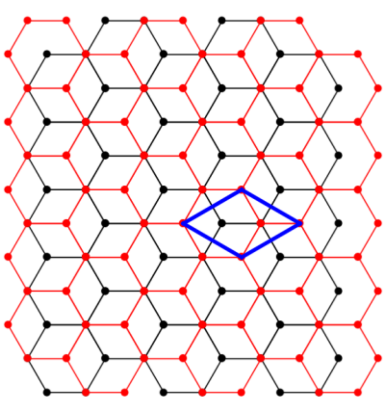

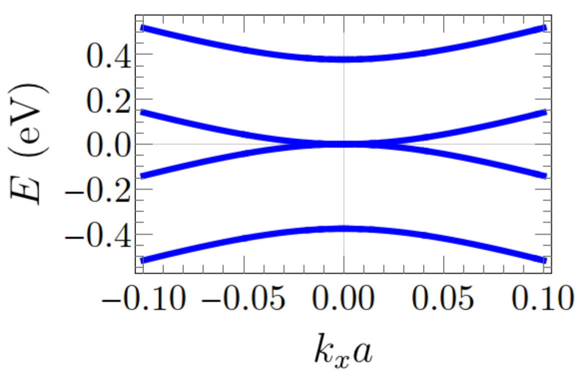

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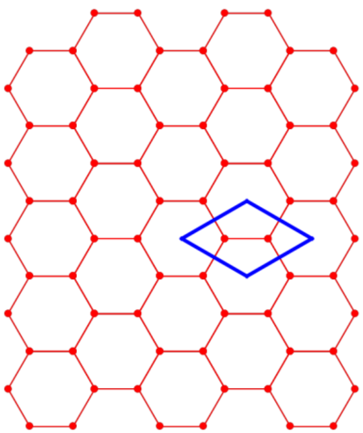

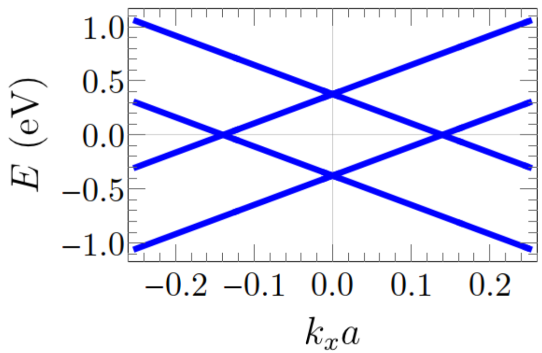

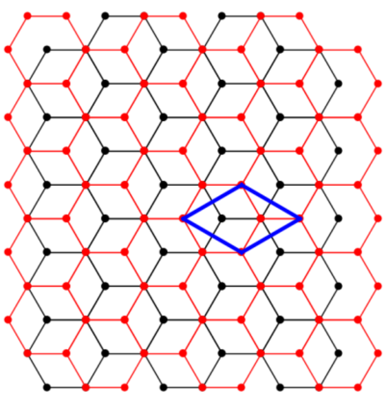

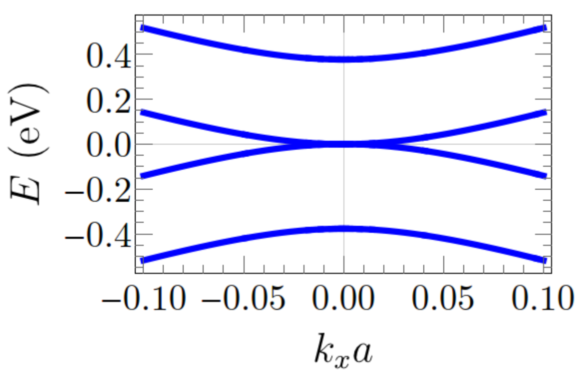

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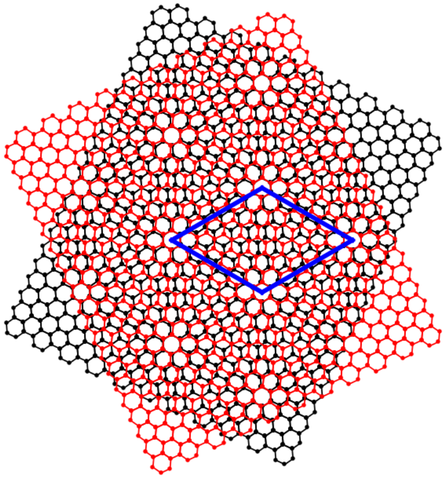

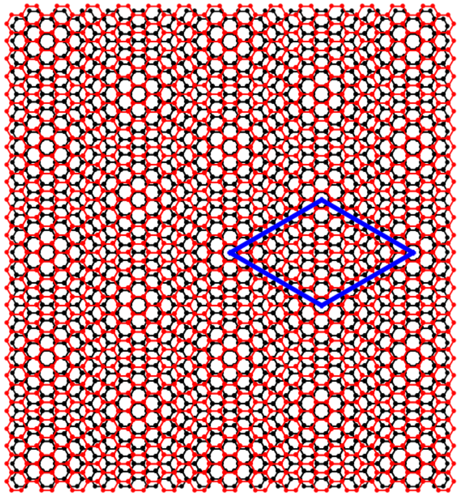

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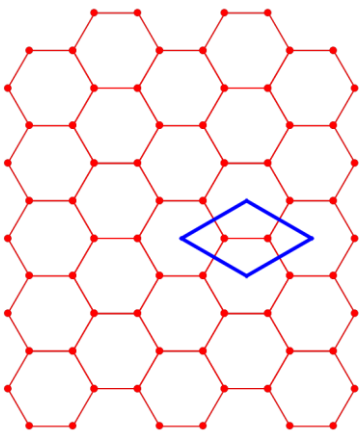

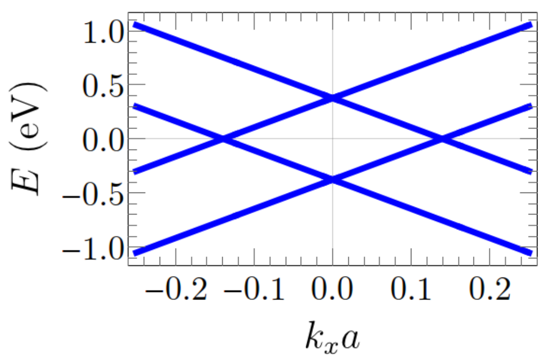

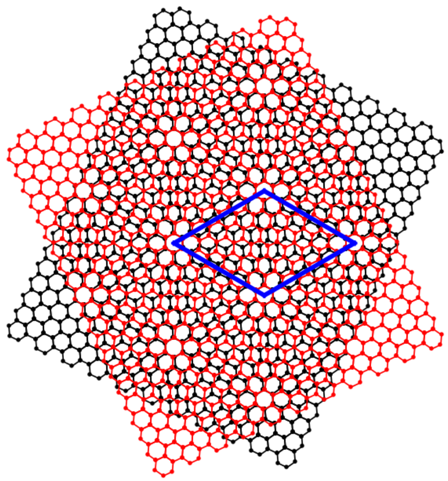

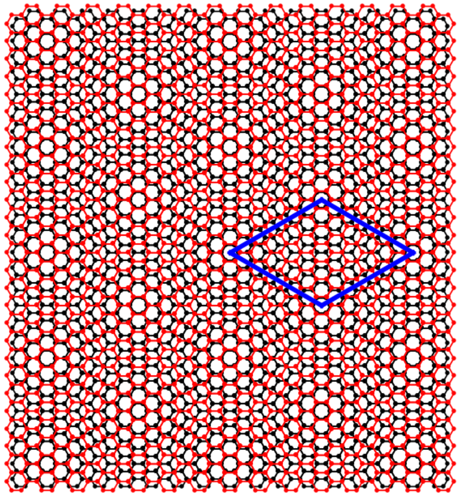

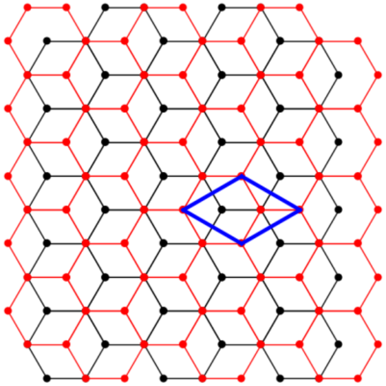

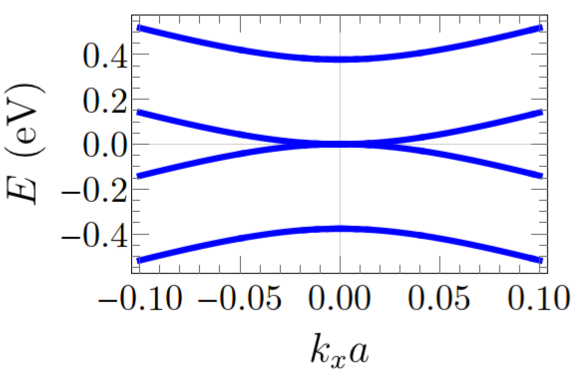

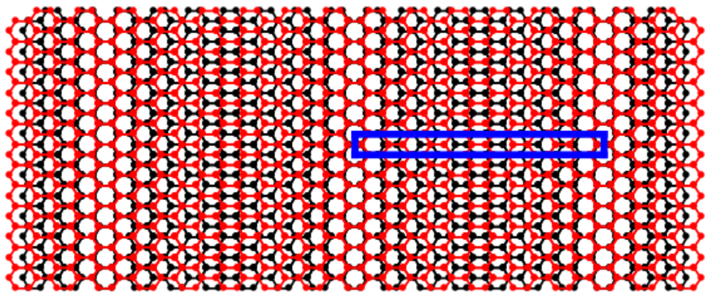

Theory

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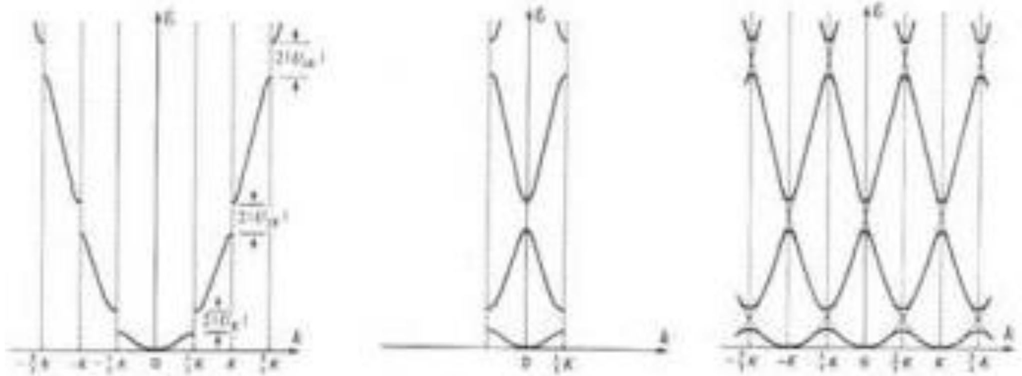

Extended-Zone Scheme

Reduced-Zone Scheme

Repeated-Zone Scheme

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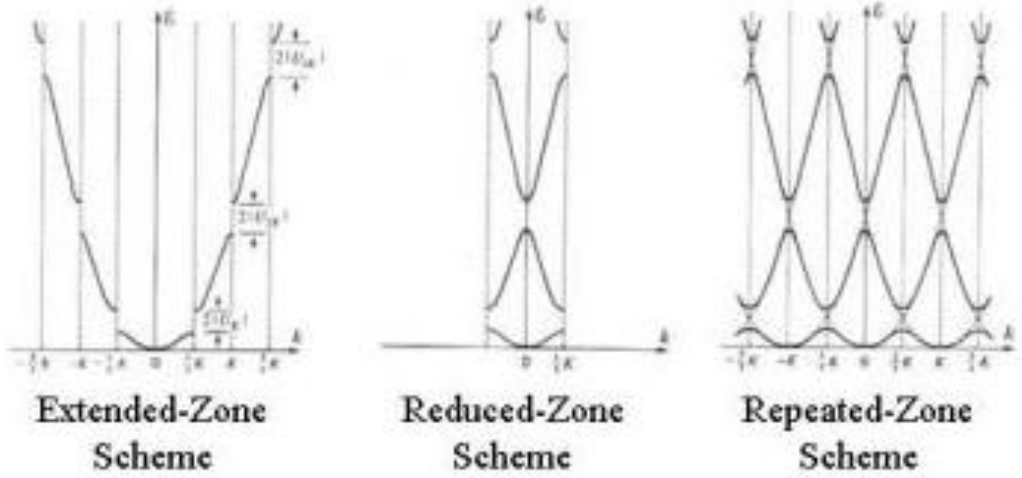
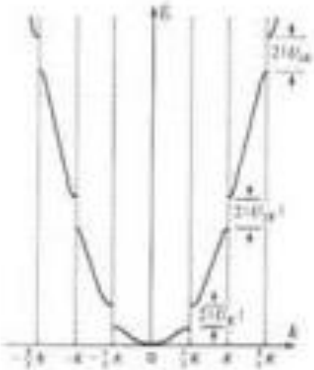
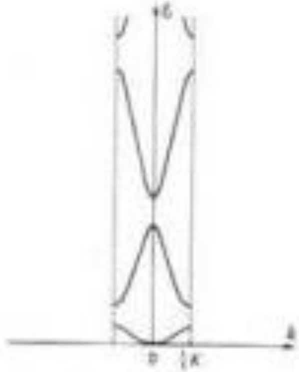


Theory

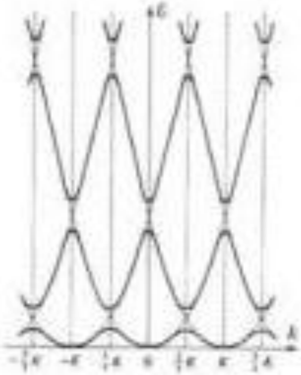
- $$\left(\hat{H}_0^b + \hat{H}_0^t + \hat{U}\right)|\Psi_{\boldsymbol{k}}\rangle = E_{\boldsymbol{k}}|\Psi_{\boldsymbol{k}}\rangle$$



Extended-Zone Scheme



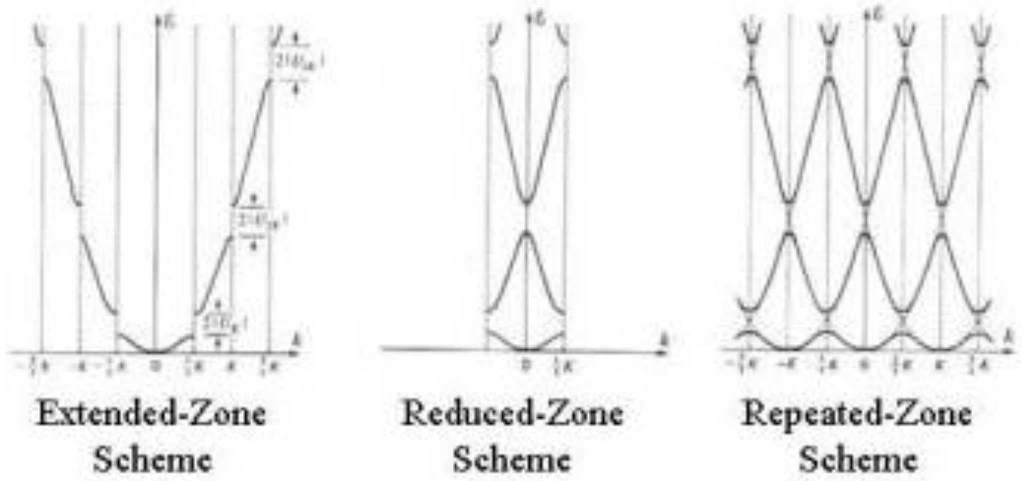
Reduced-Zone Scheme



Repeated-Zone Scheme

Theory

- $$\left(\hat{H}_0^b + \hat{H}_0^t + \hat{U}\right)|\Psi_{\boldsymbol{k}}\rangle = E_{\boldsymbol{k}}|\Psi_{\boldsymbol{k}}\rangle$$



- Insert a complete basis of Bloch states of the individual layers $|\Phi_{\boldsymbol{\kappa}}^{i,\chi}\rangle$

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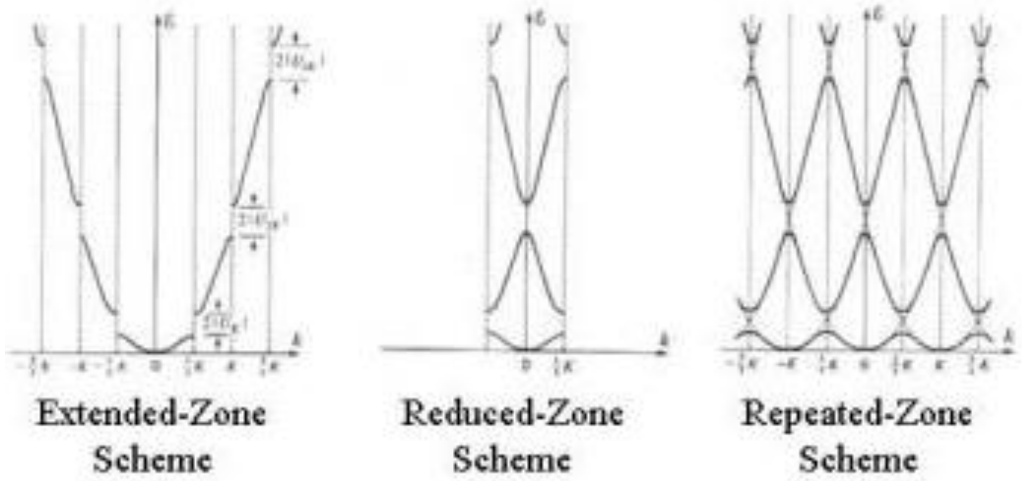

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$$\sum_{\chi'}\left(\left[H_0^b(\boldsymbol{k}+\boldsymbol{G})\right]_{\chi,\chi'} C_{\boldsymbol{G}}^{b,\chi'}(\boldsymbol{k}) + \sum_{\boldsymbol{G}'\in BZ^{(t)}} U_{\boldsymbol{G},\boldsymbol{G}'}^{\chi,\chi'}(\boldsymbol{k}) C_{\boldsymbol{G}'}^{t,\chi'}(\boldsymbol{k})\right) = E_{\boldsymbol{k}} C_{\boldsymbol{G}}^{b,\chi}(\boldsymbol{k})$$

$$\sum_{\chi'}\left(\left[H_0^t(\boldsymbol{k}+\boldsymbol{G})\right]_{\chi,\chi'} C_{\boldsymbol{G}}^{t,\chi'}(\boldsymbol{k}) + \sum_{\boldsymbol{G}'\in BZ^{(b)}} \left(U_{\boldsymbol{G},\boldsymbol{G}'}^{\chi,\chi'}\right)^*(\boldsymbol{k}) C_{\boldsymbol{G}'}^{b,\chi'}(\boldsymbol{k})\right) = E_{\boldsymbol{k}} C_{\boldsymbol{G}}^{t,\chi}(\boldsymbol{k})$$

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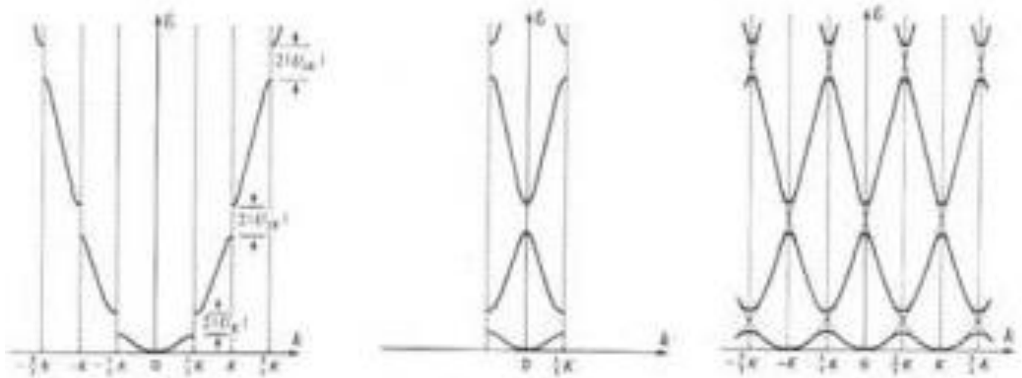

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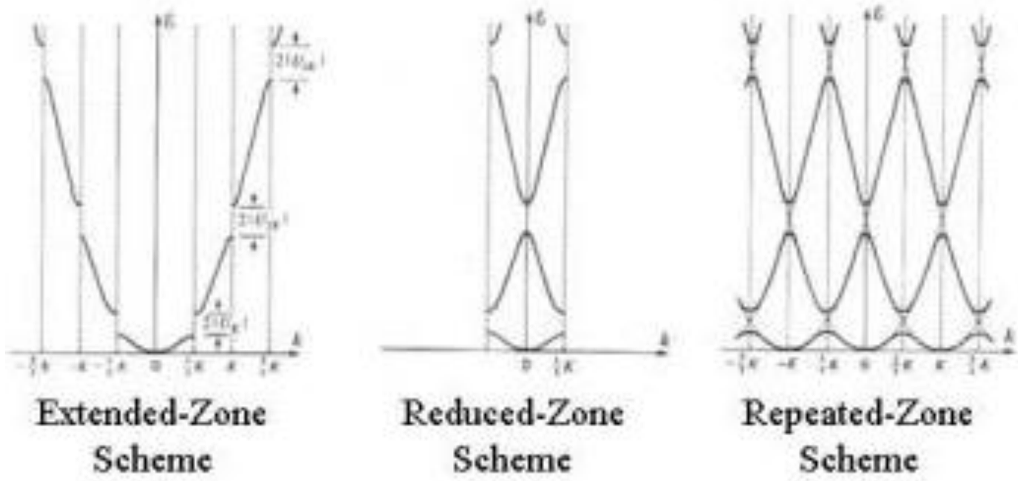

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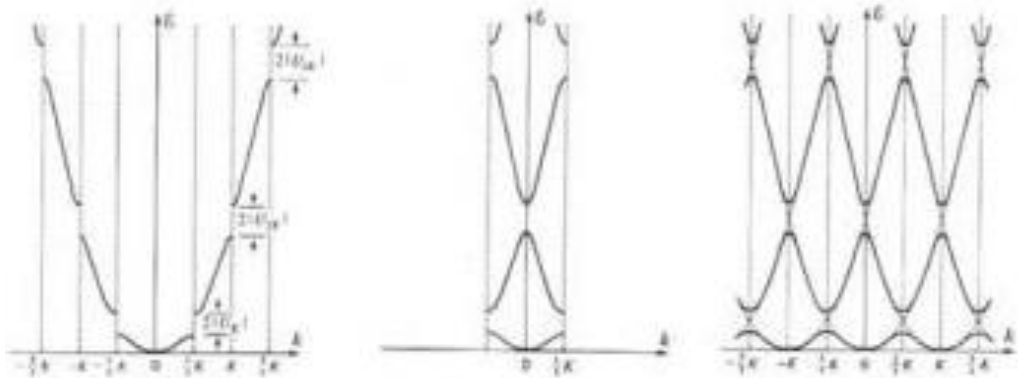

Extended-Zone Scheme | Reduced-Zone Scheme | Repeated-Zone Scheme

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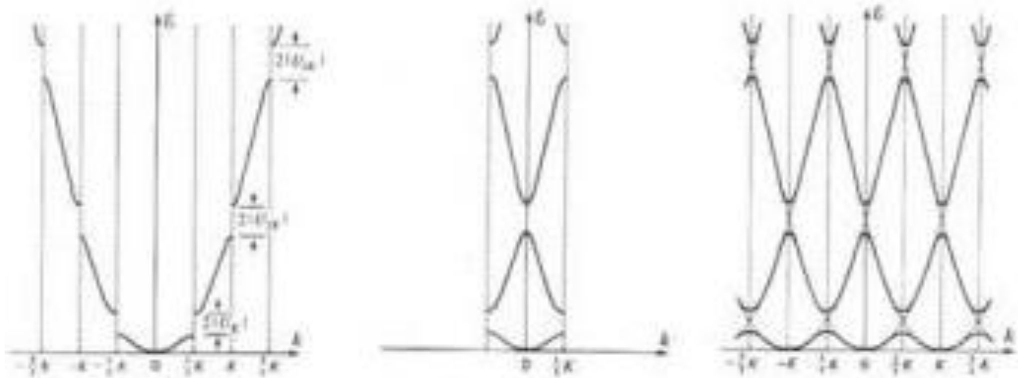

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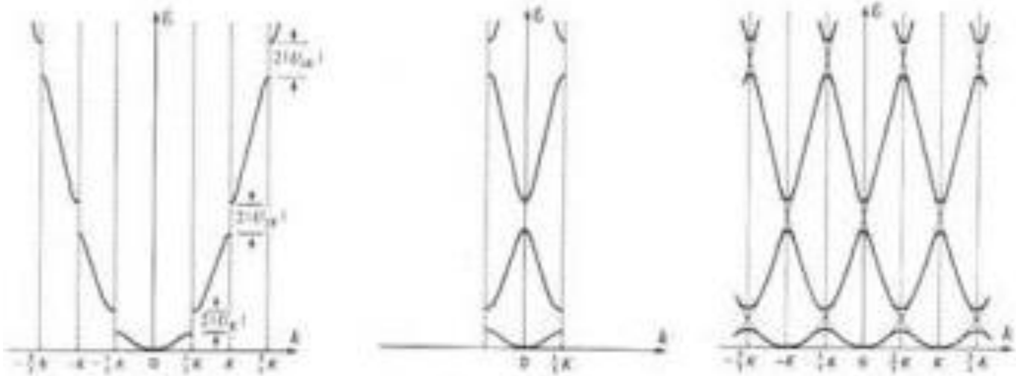

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Twisted bilayer graphene

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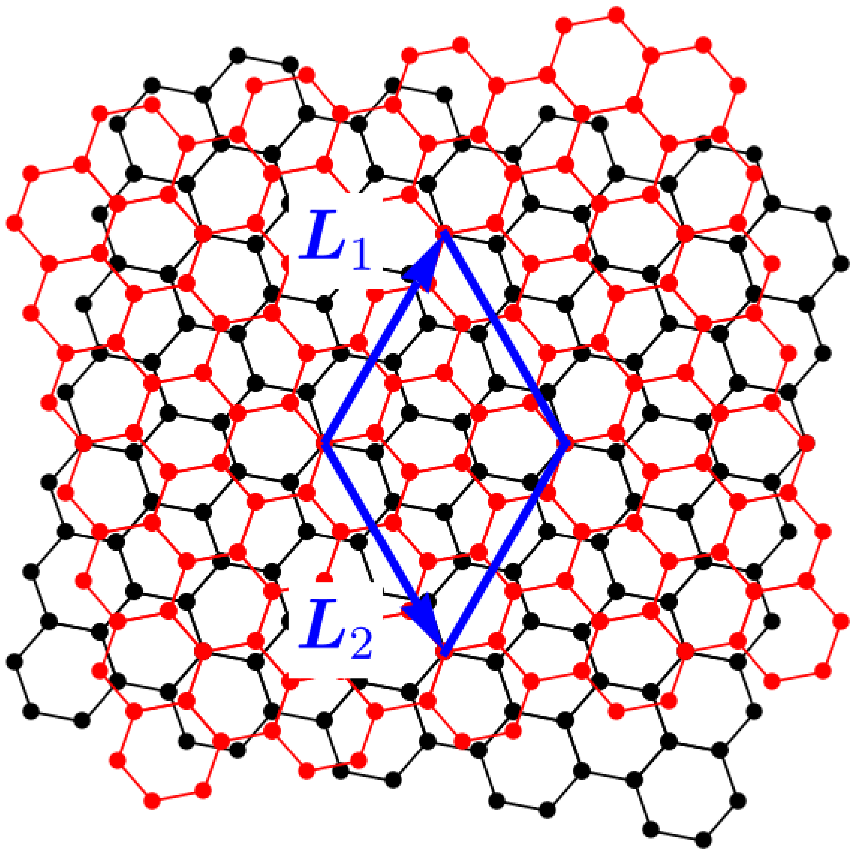

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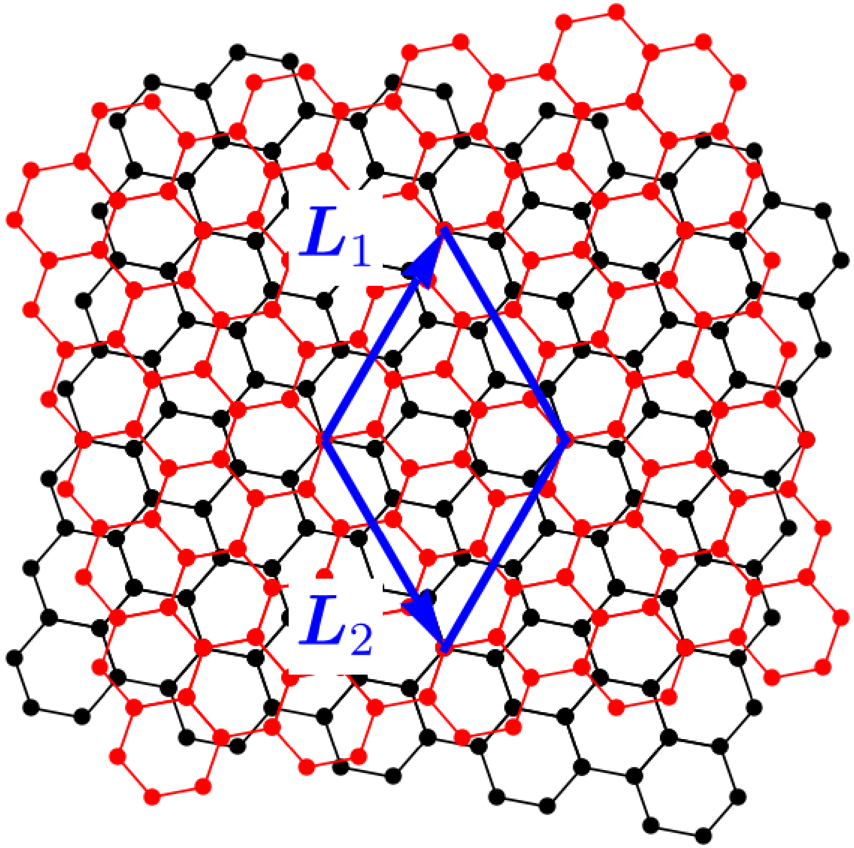
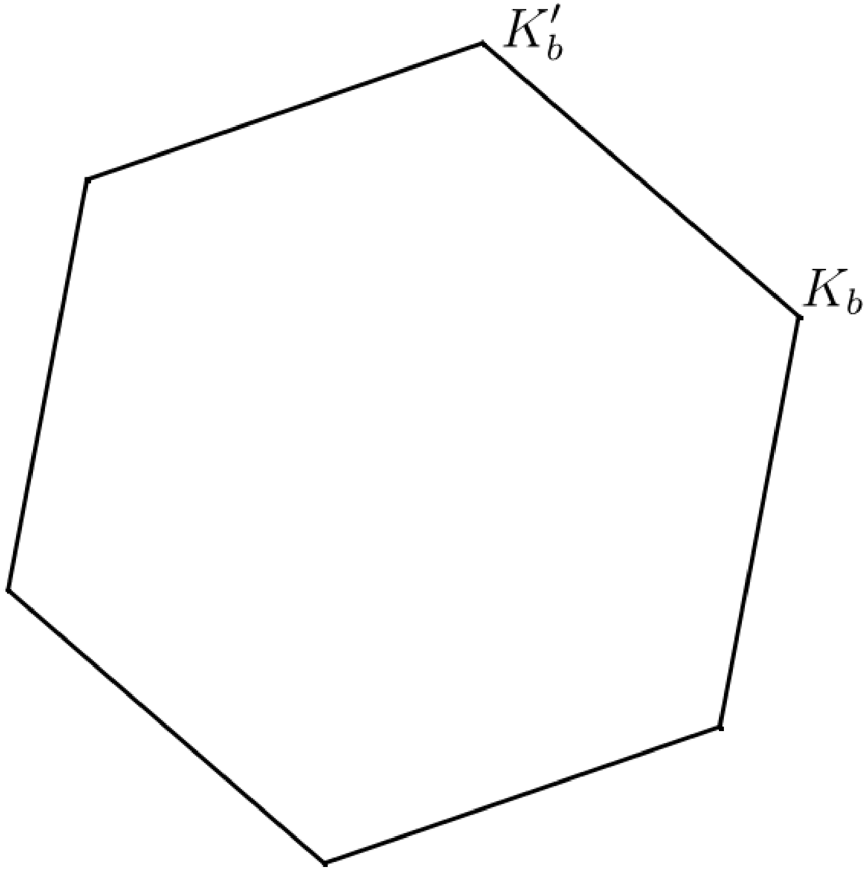
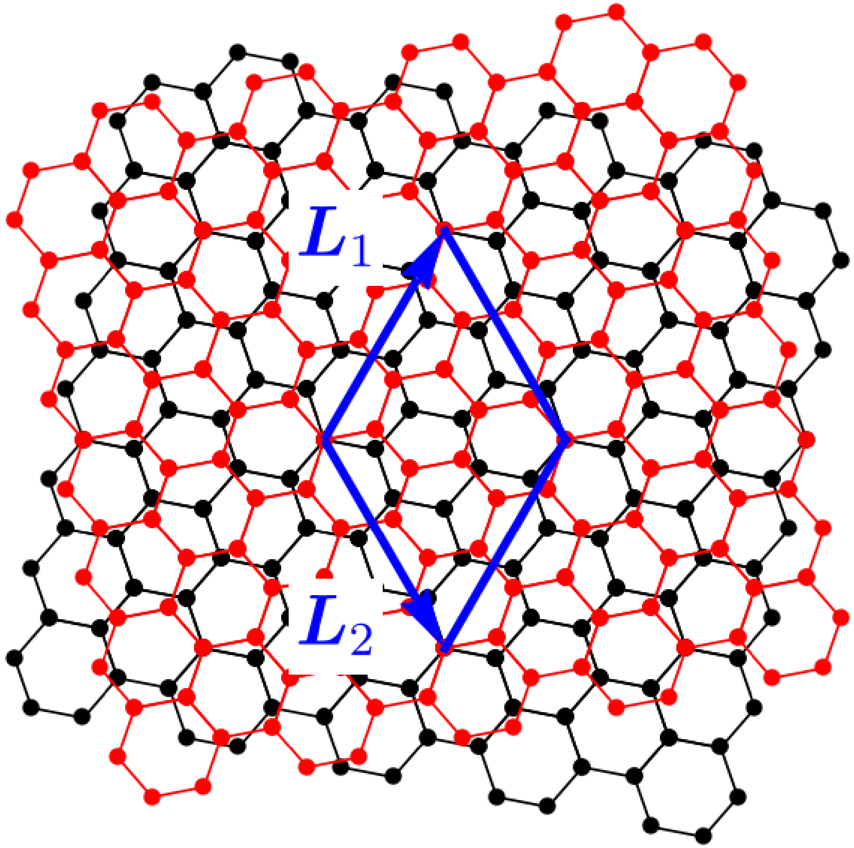
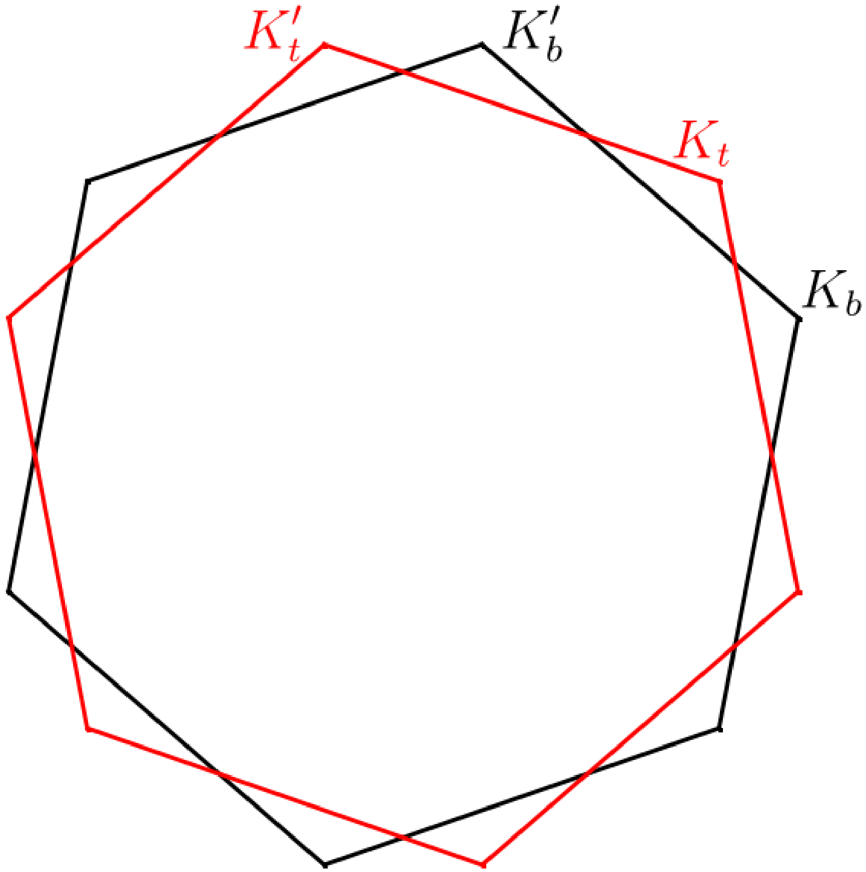




Twisted bilayer graphene





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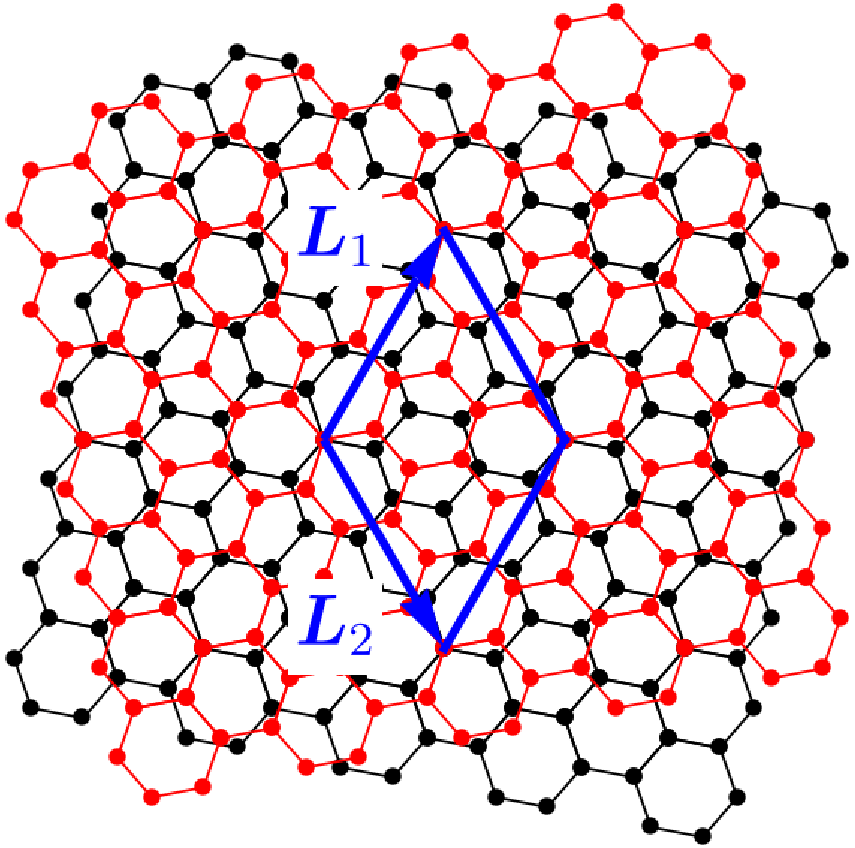

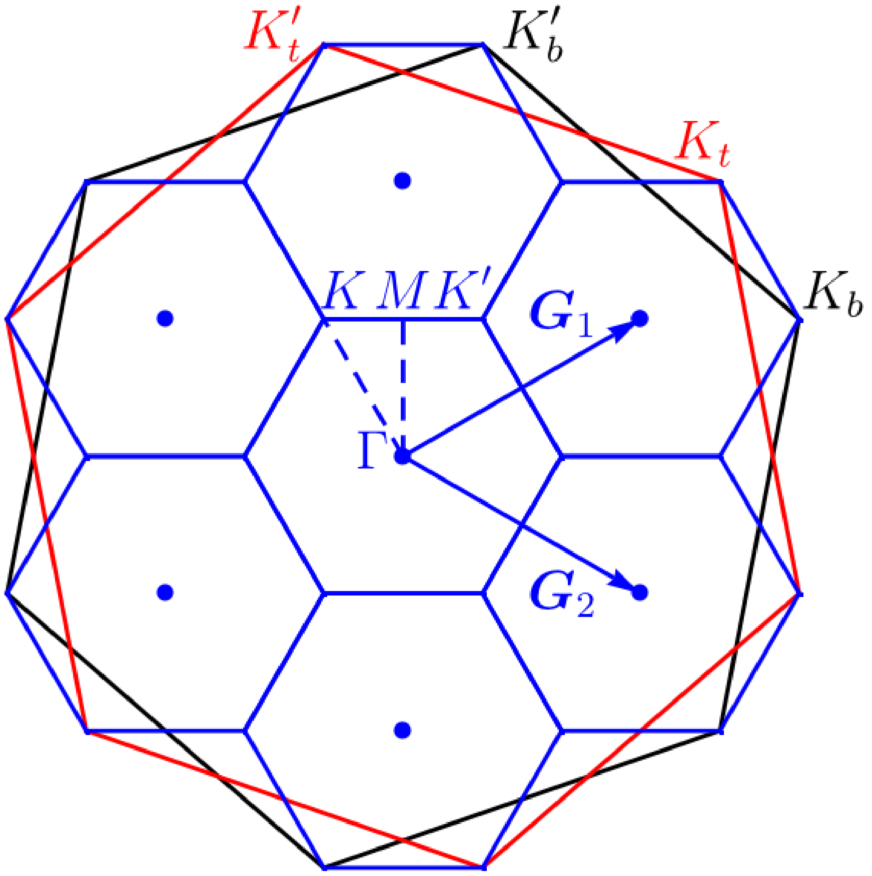

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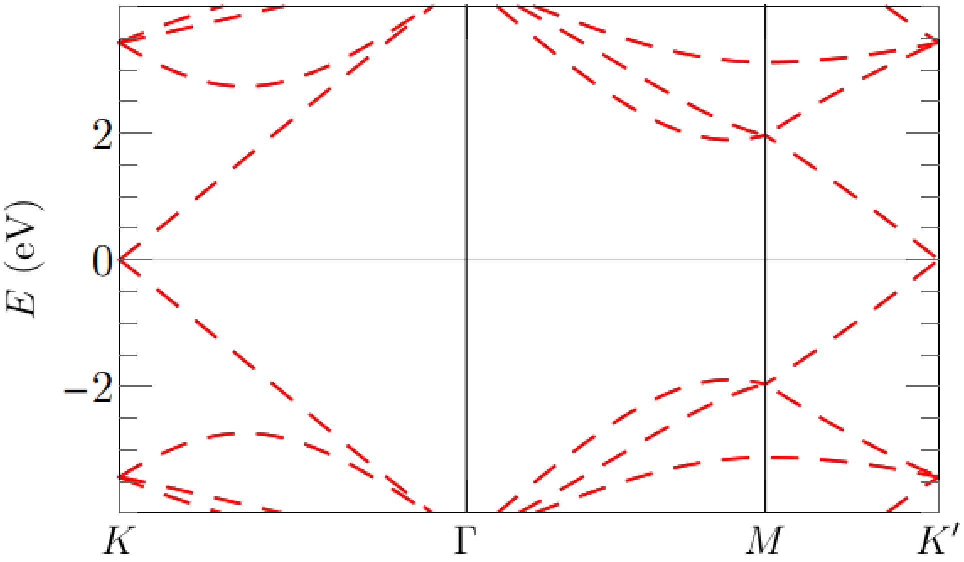

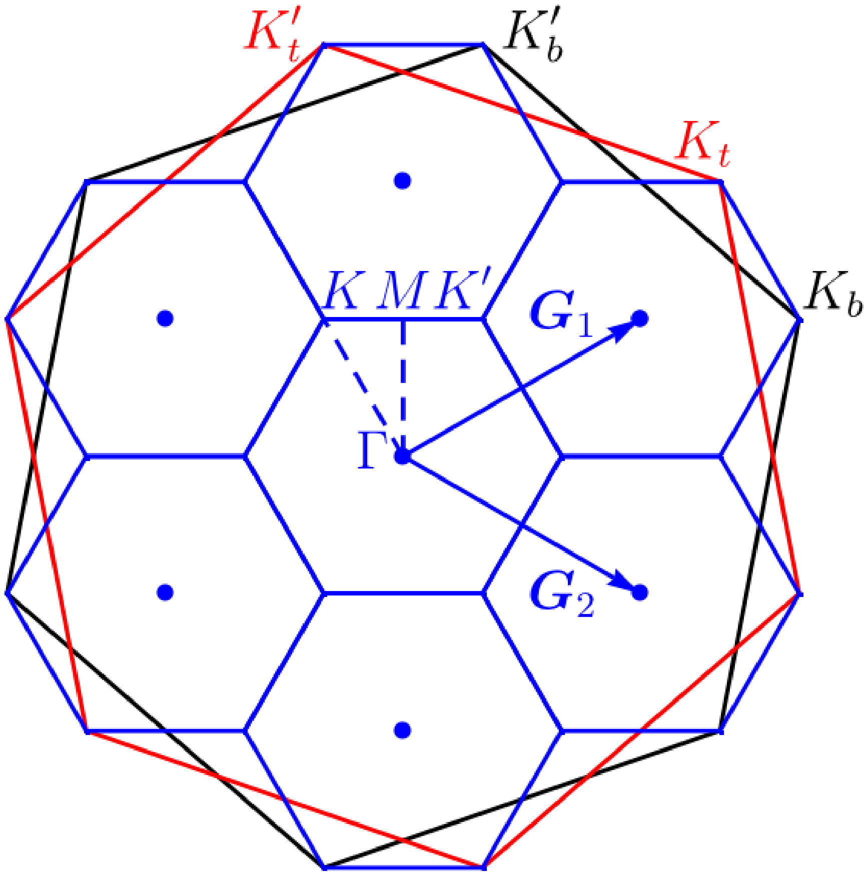

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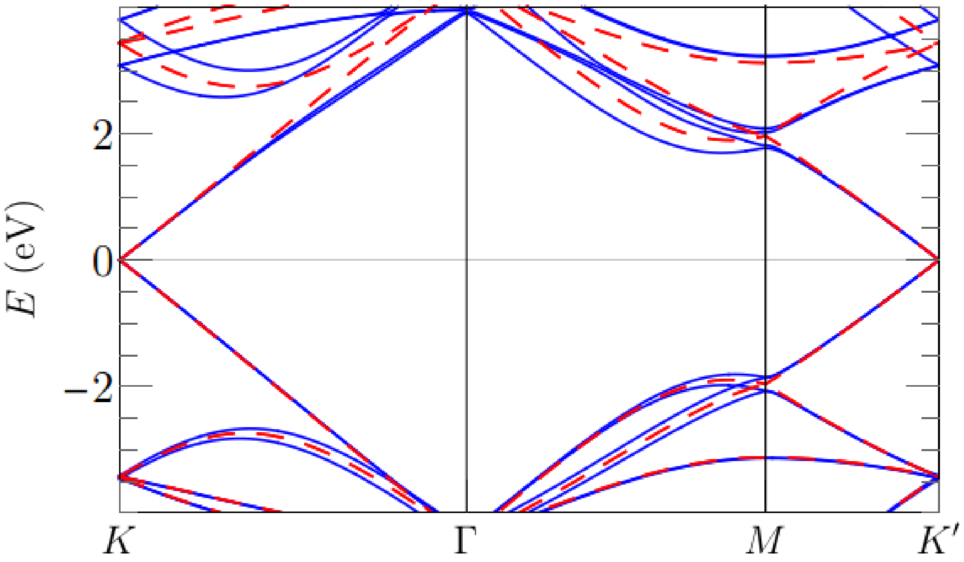

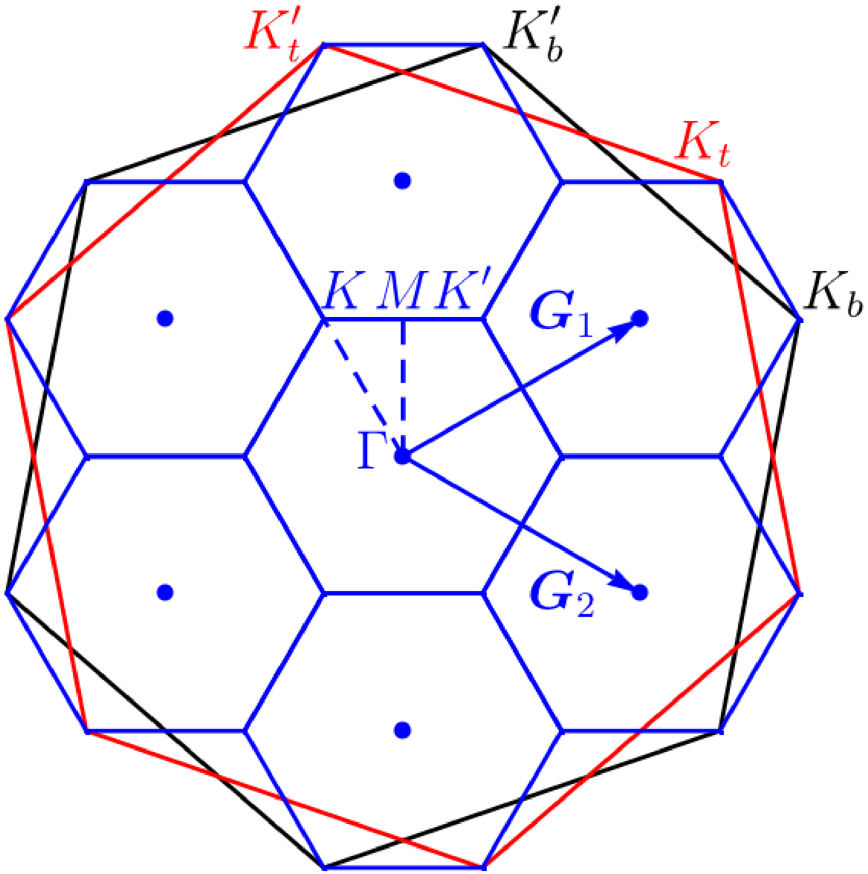

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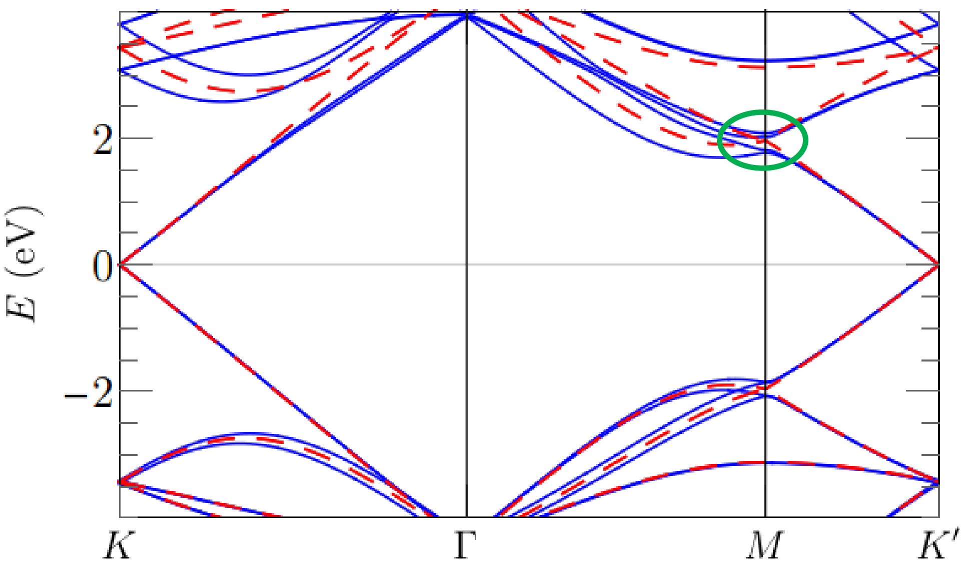

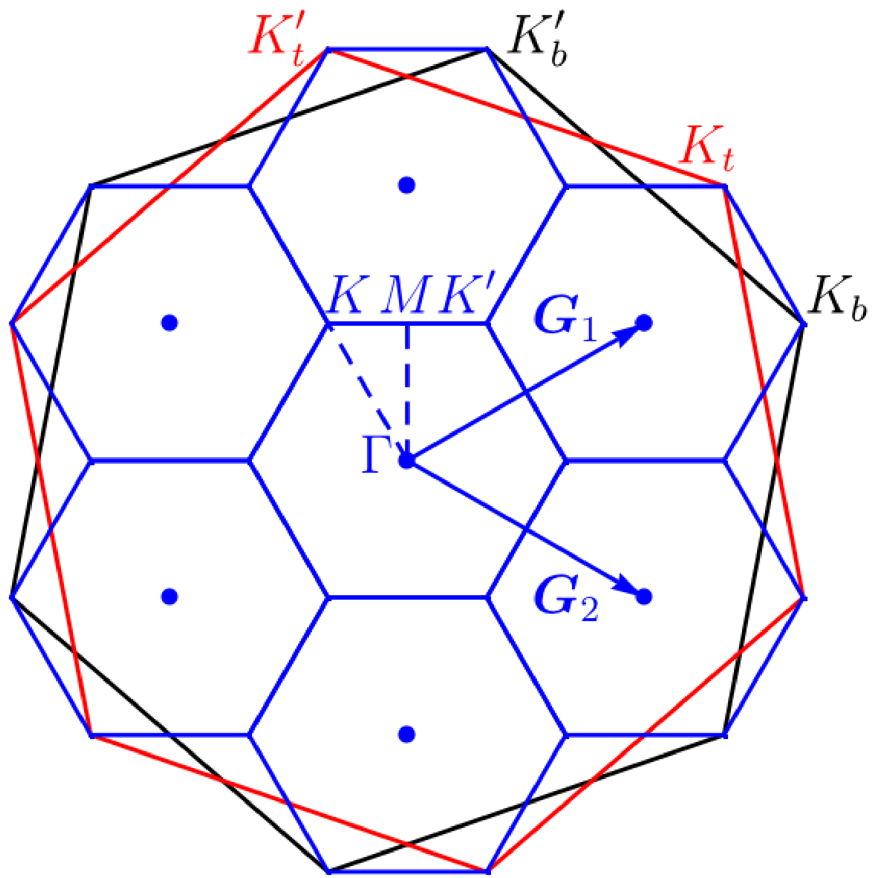

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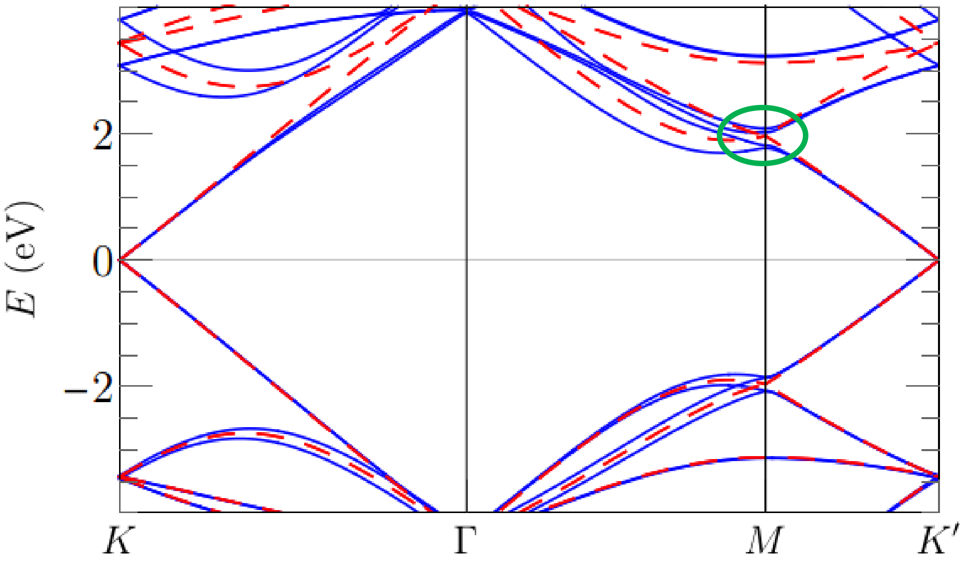

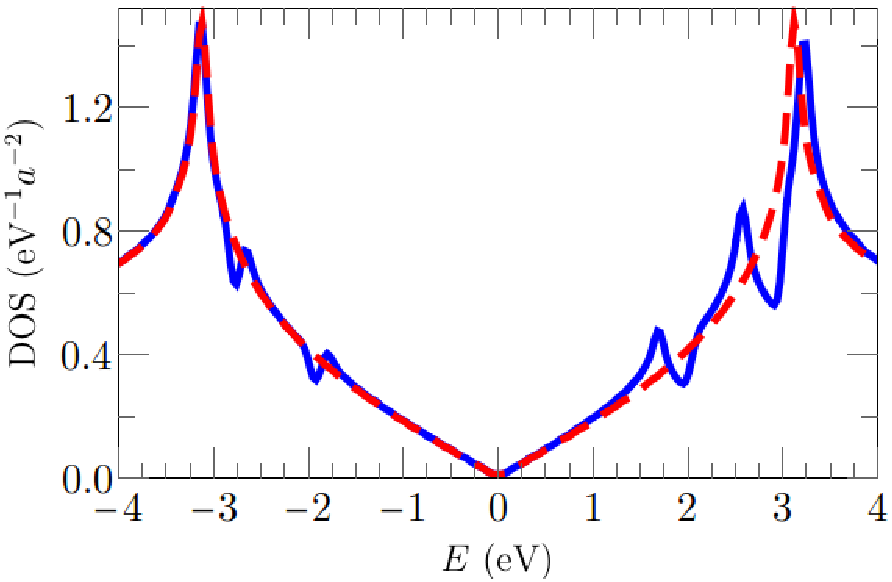

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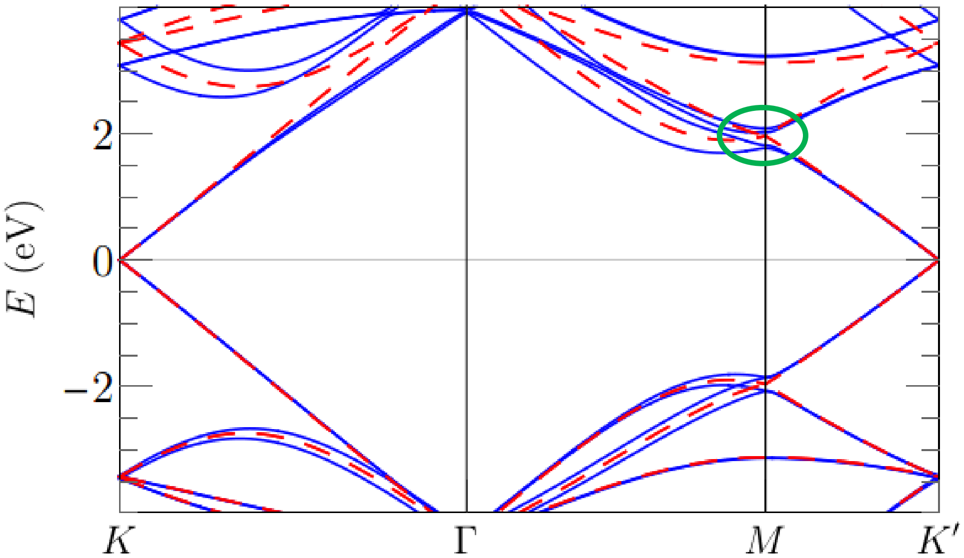

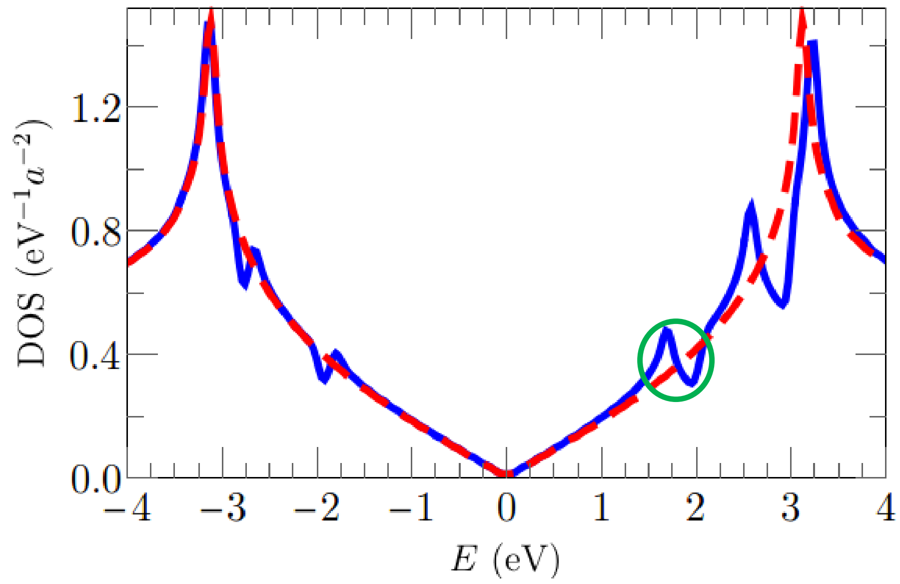

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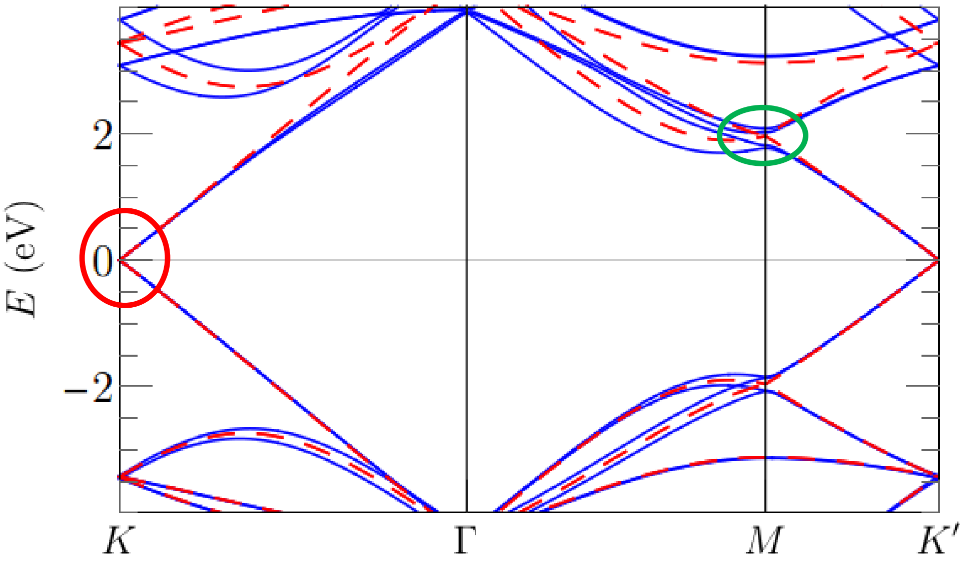
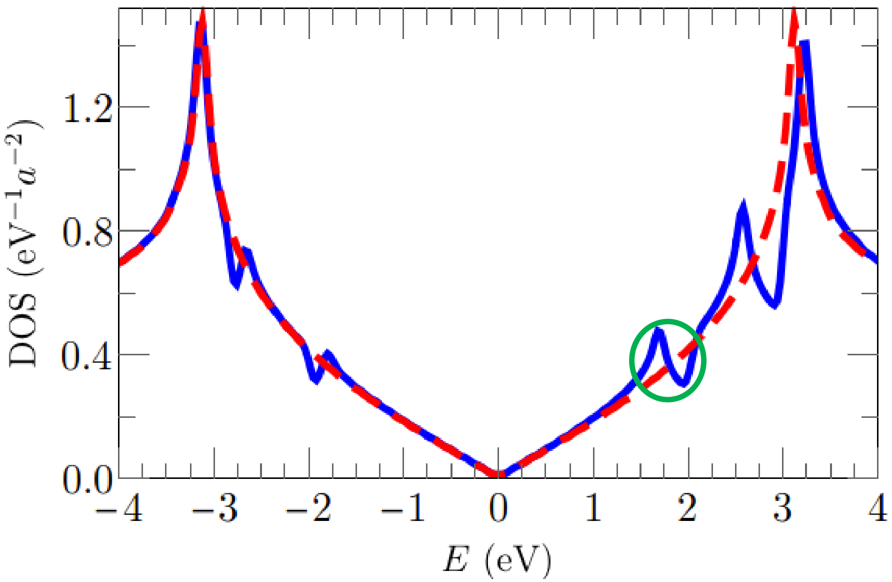
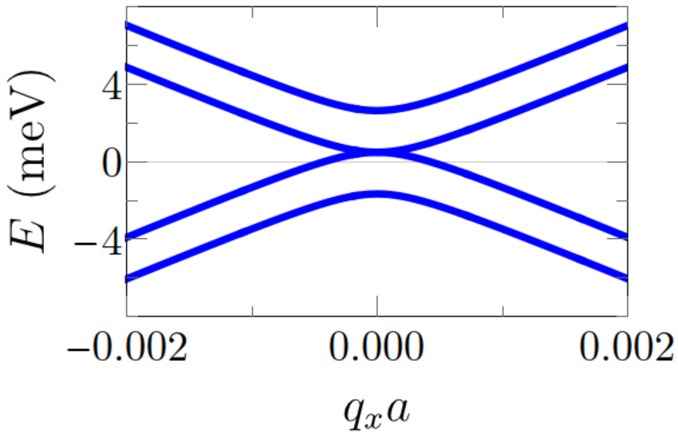




Twisted bilayer graphene

Twisted bilayer graphene



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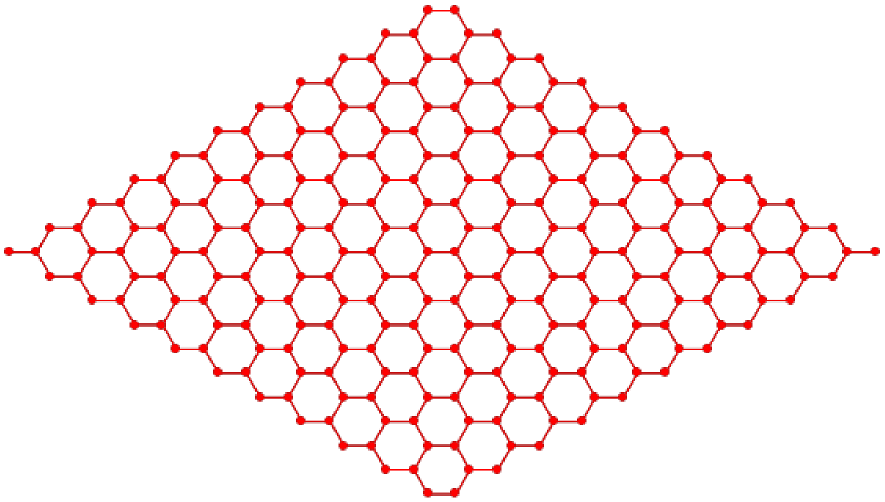

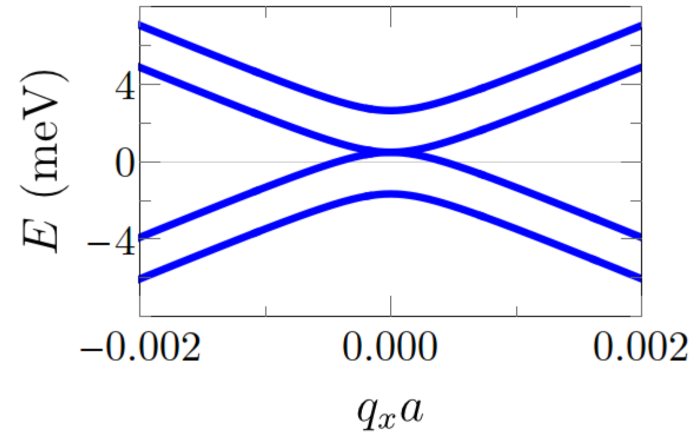

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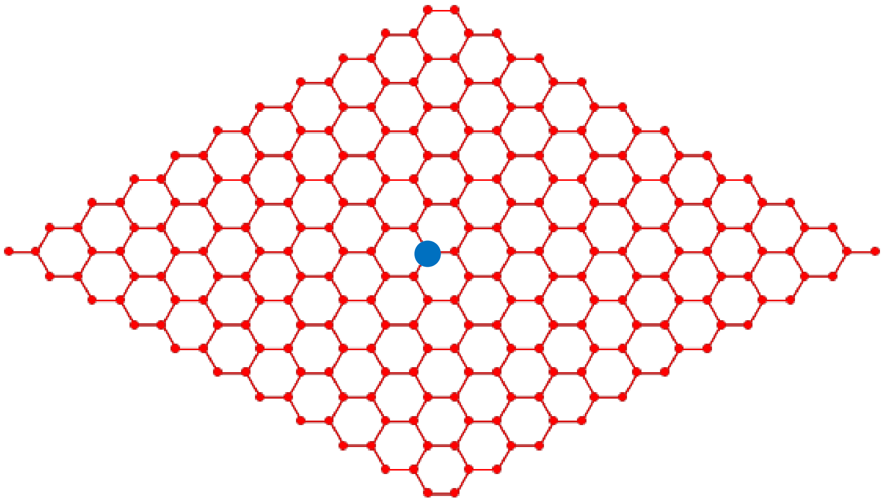

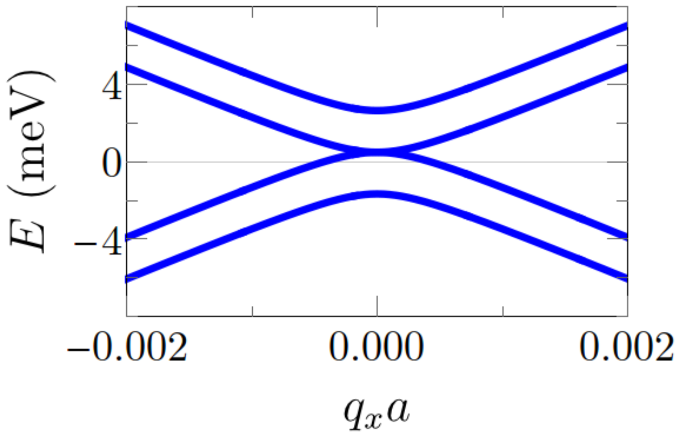

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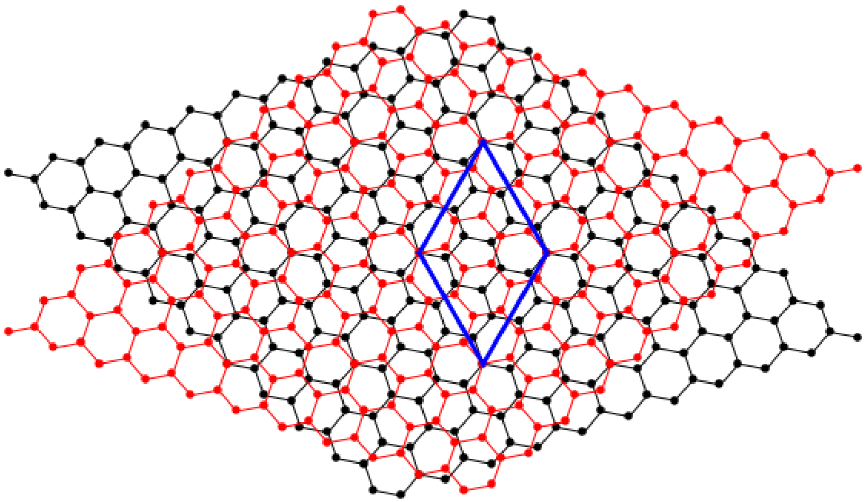

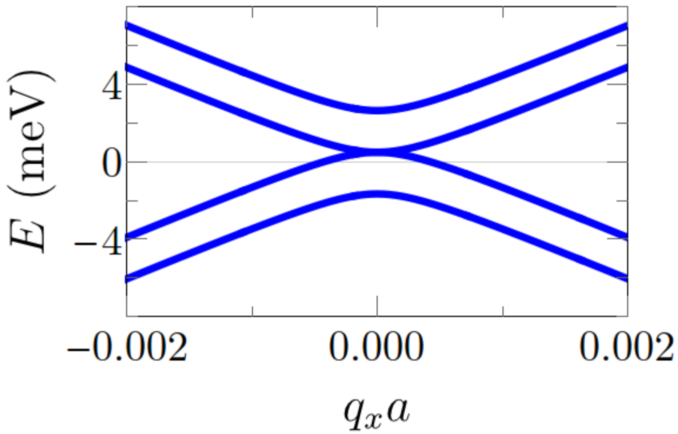

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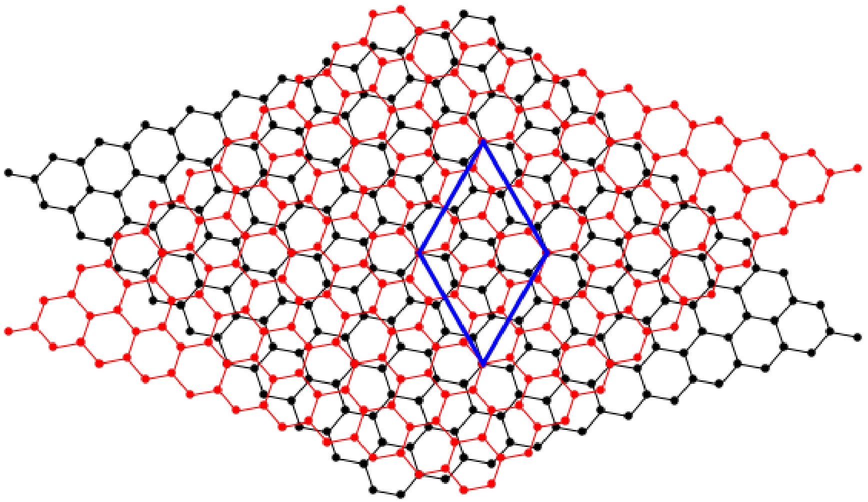

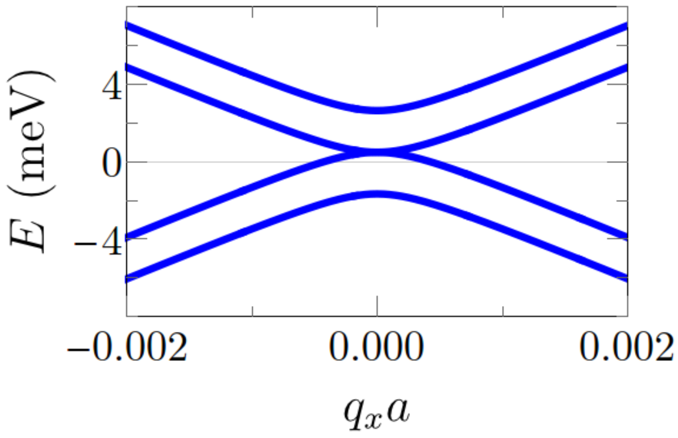

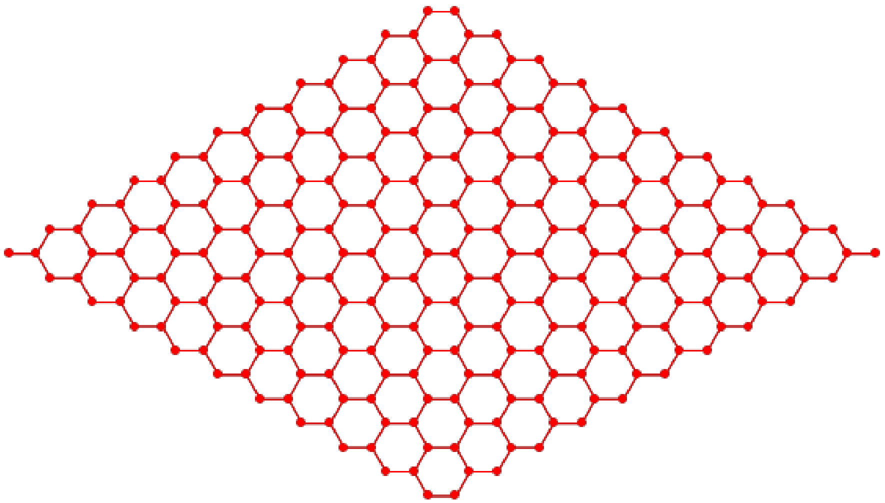

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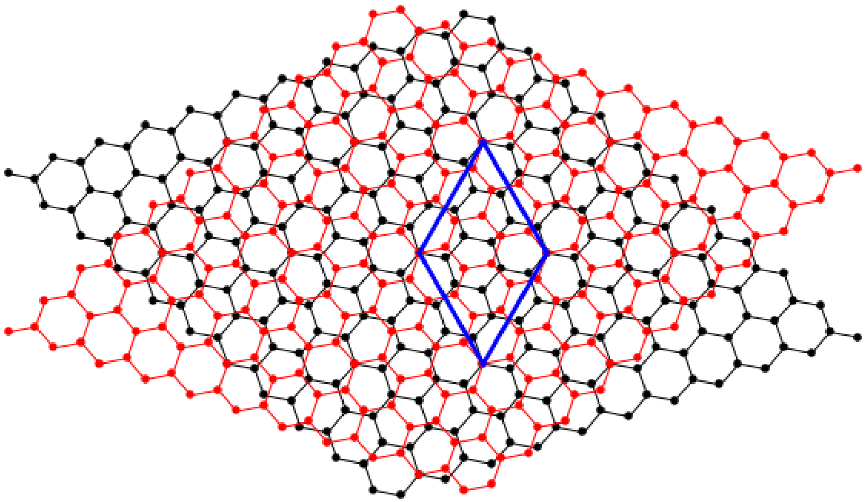

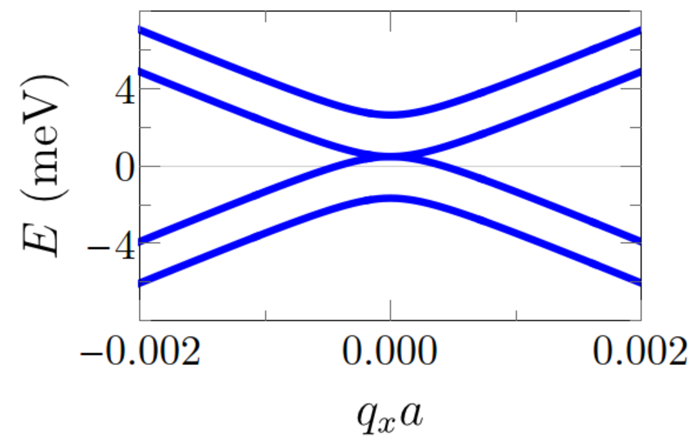

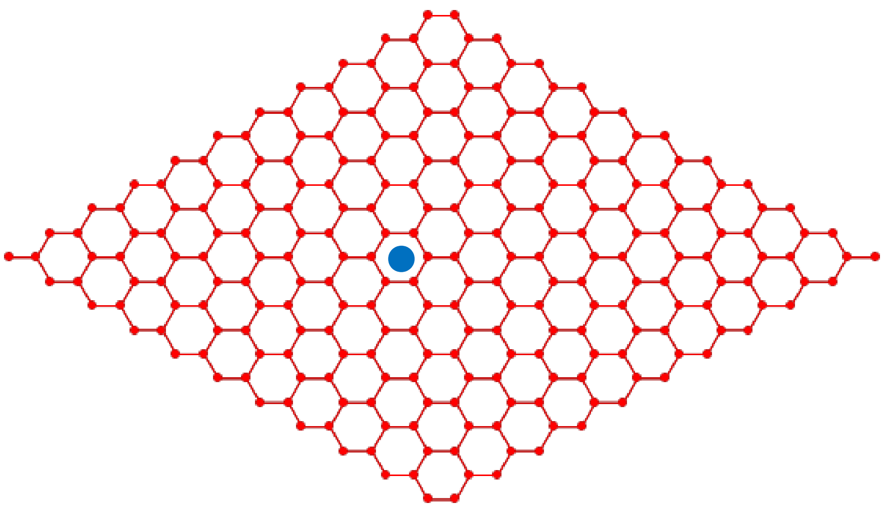

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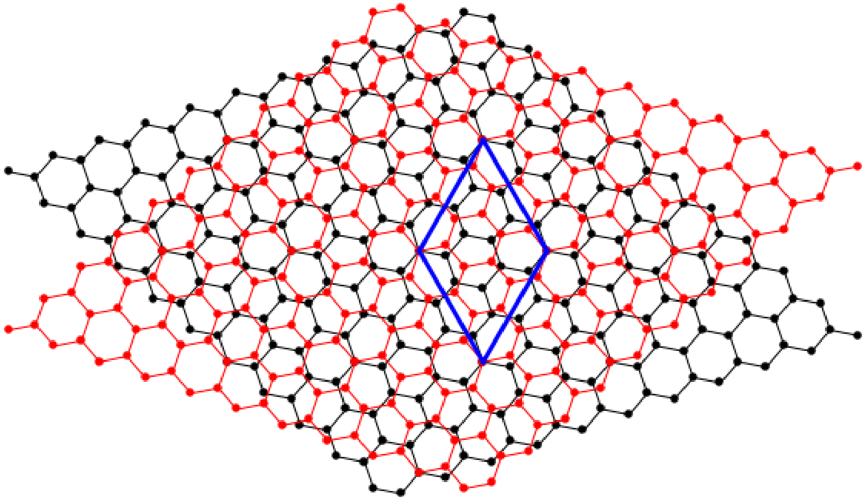

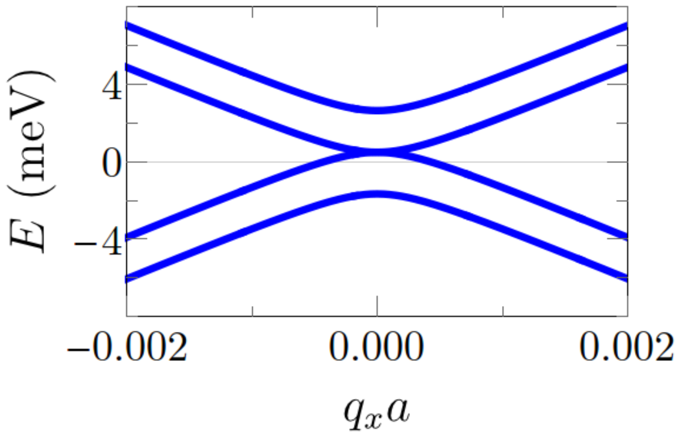

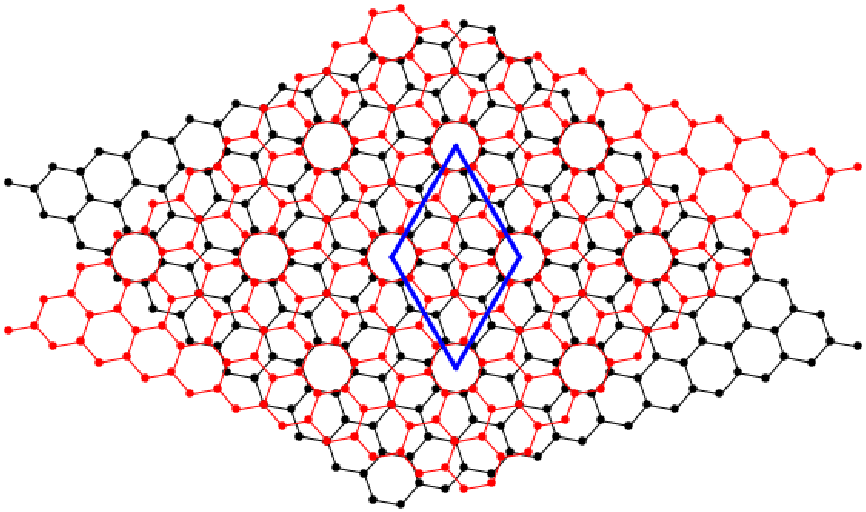

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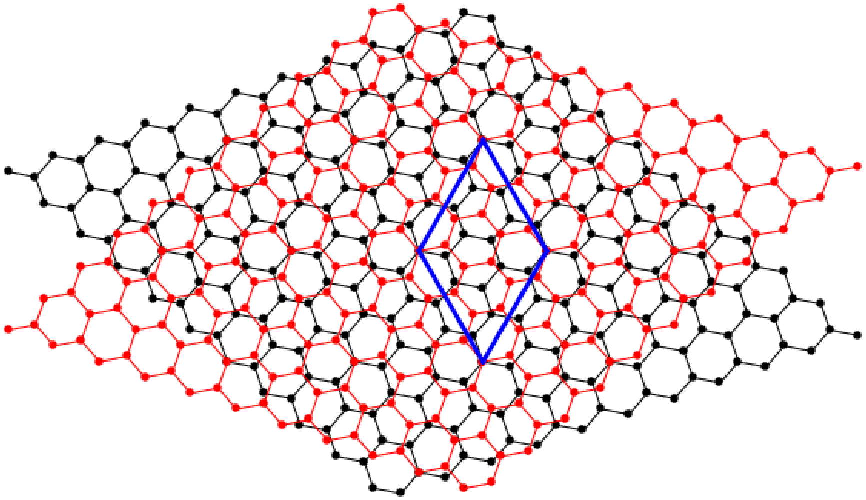

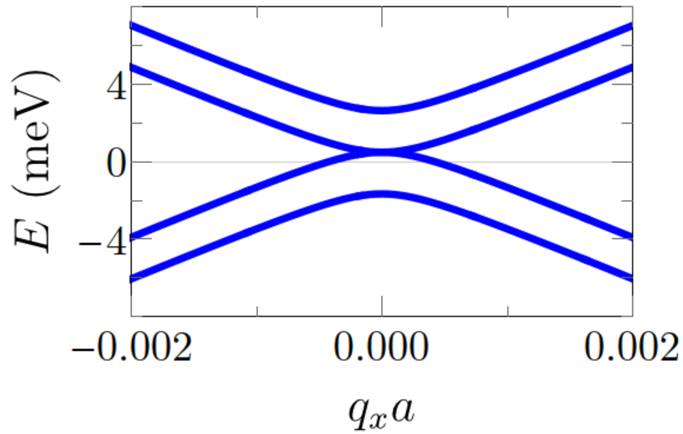

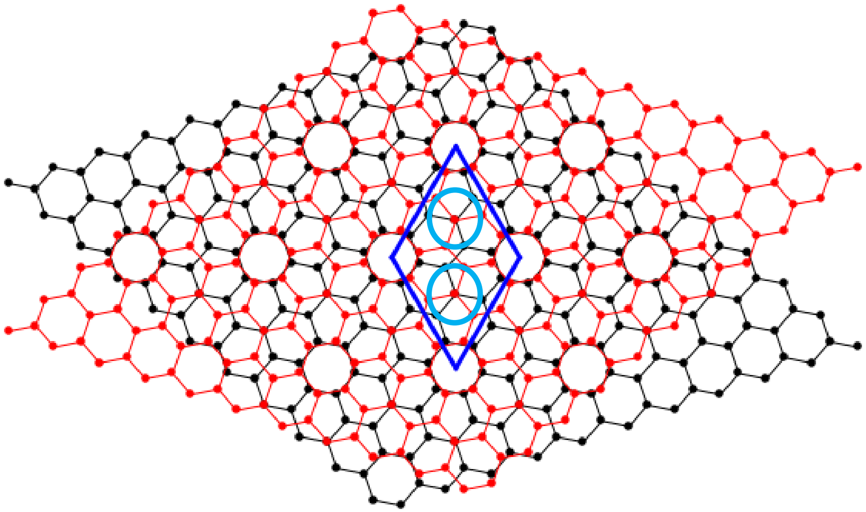

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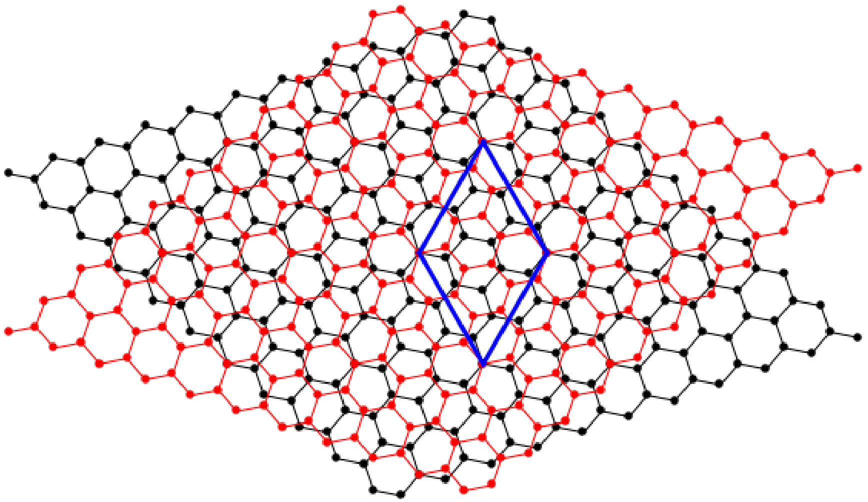

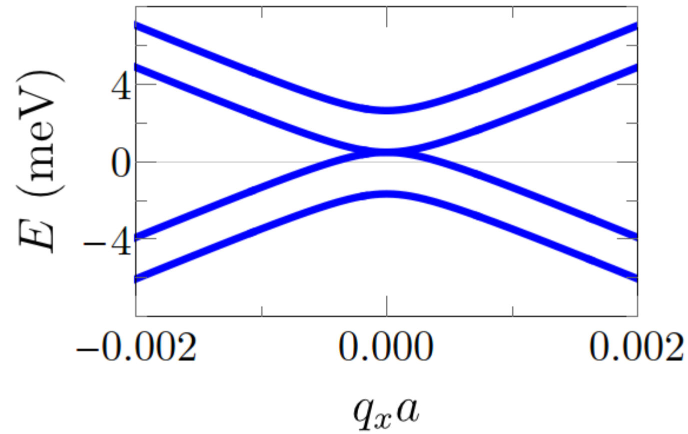

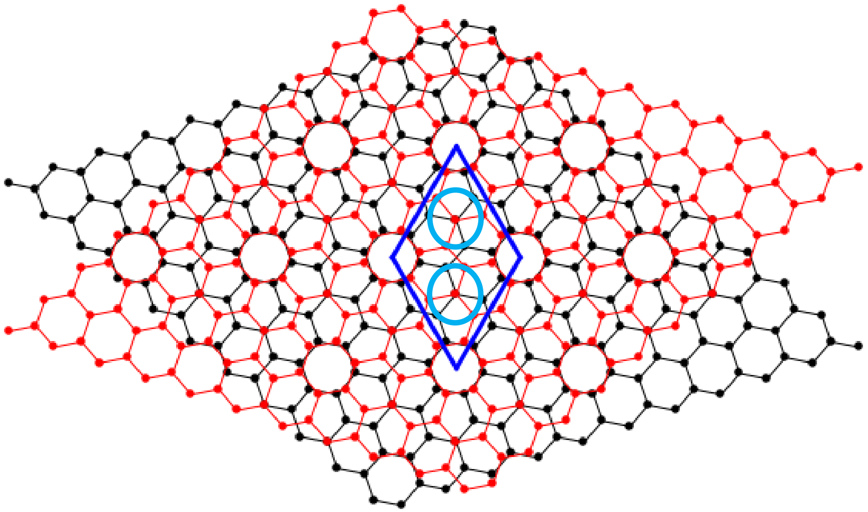

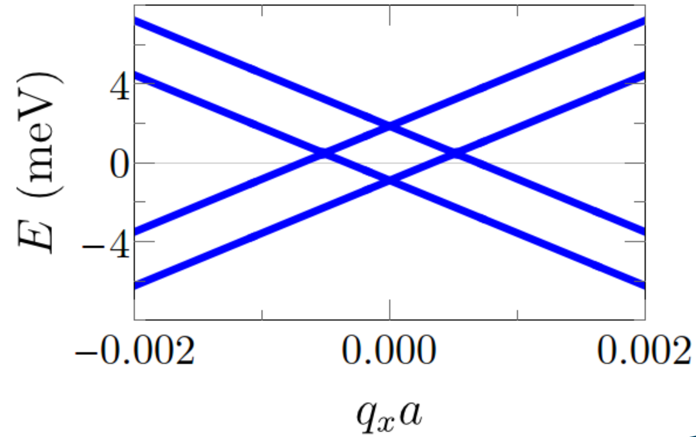

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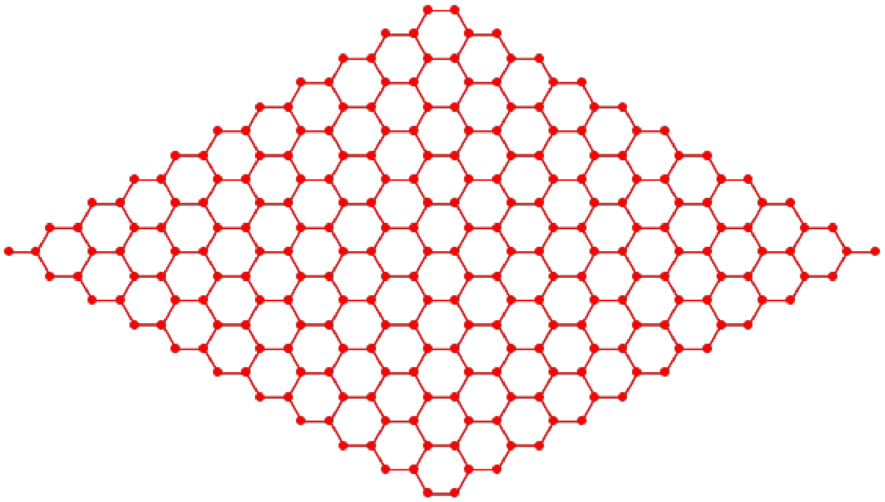

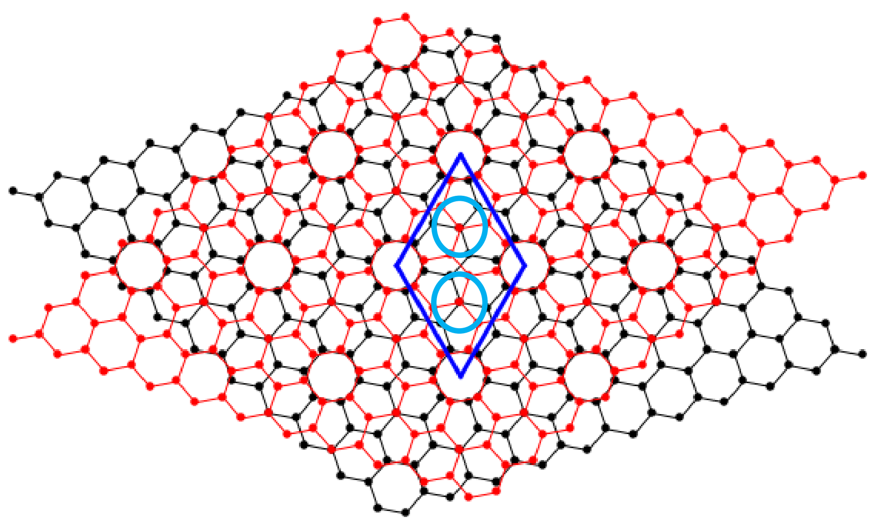

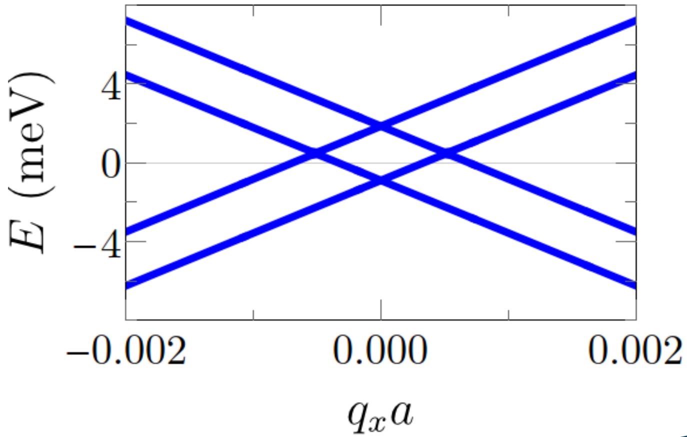

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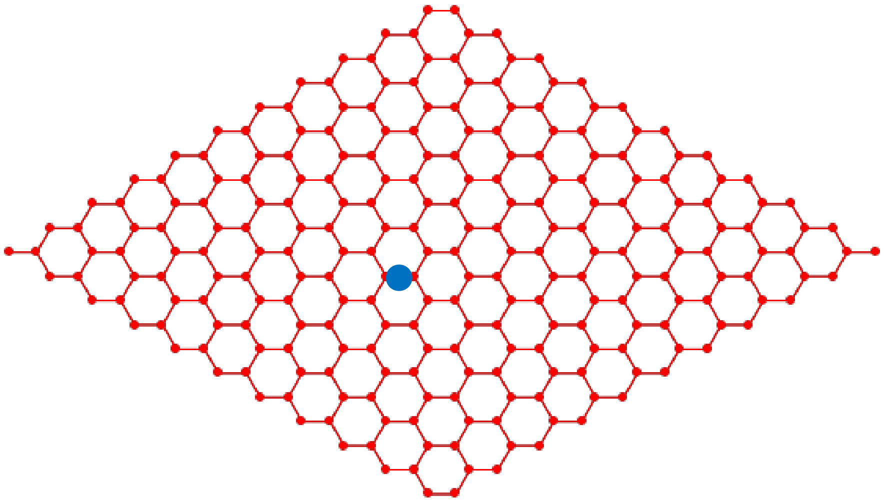

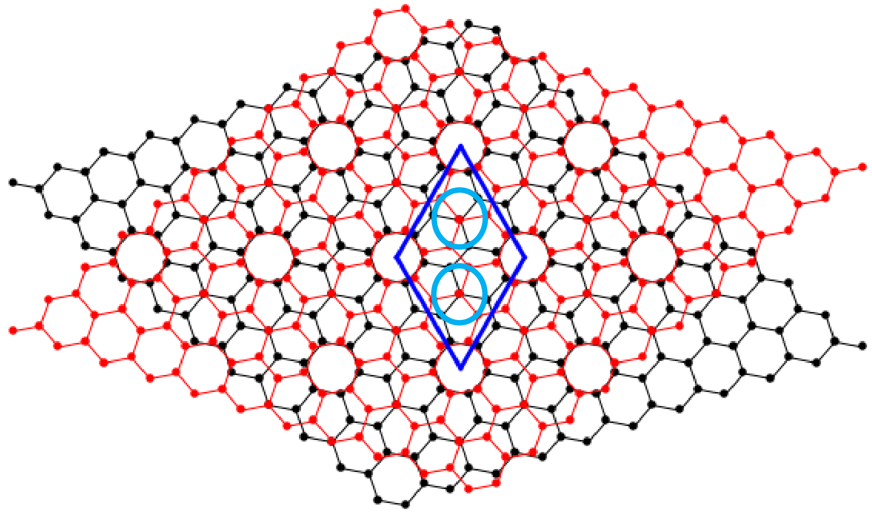

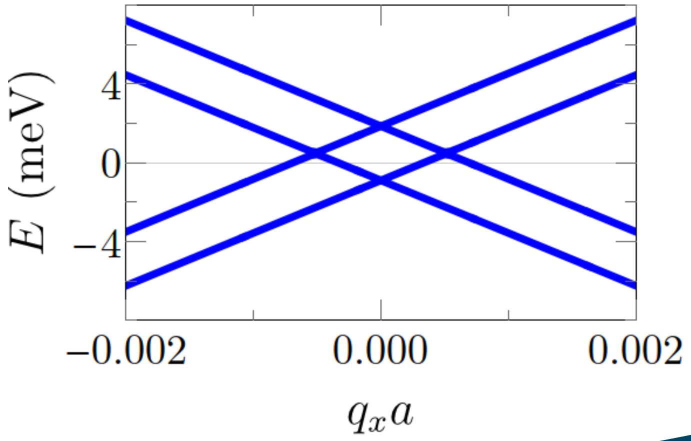

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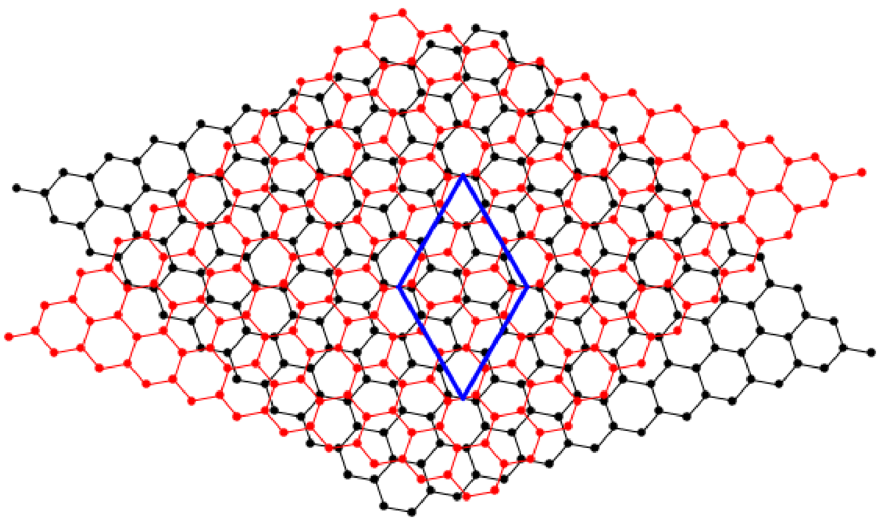

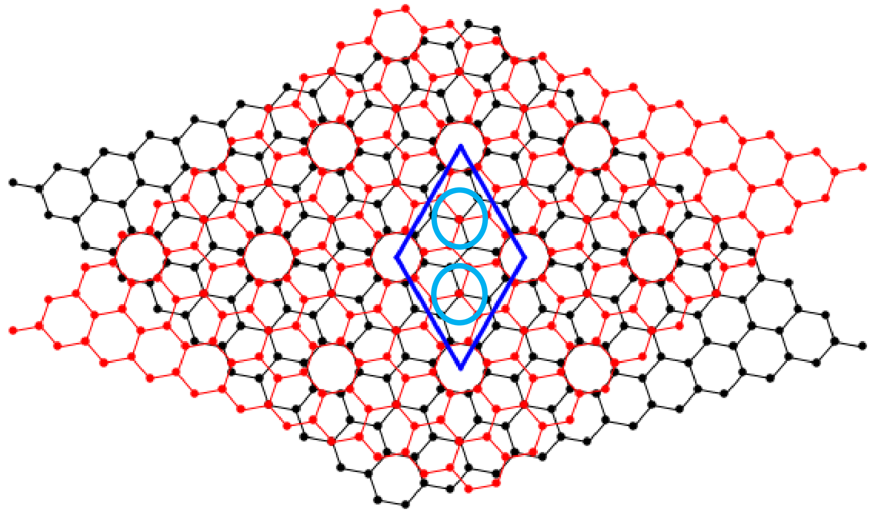

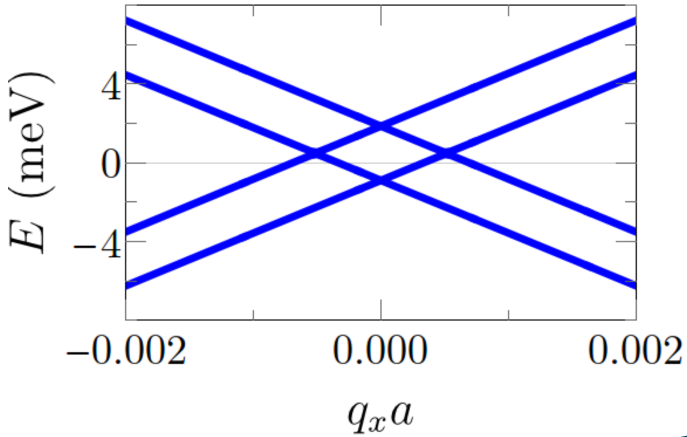

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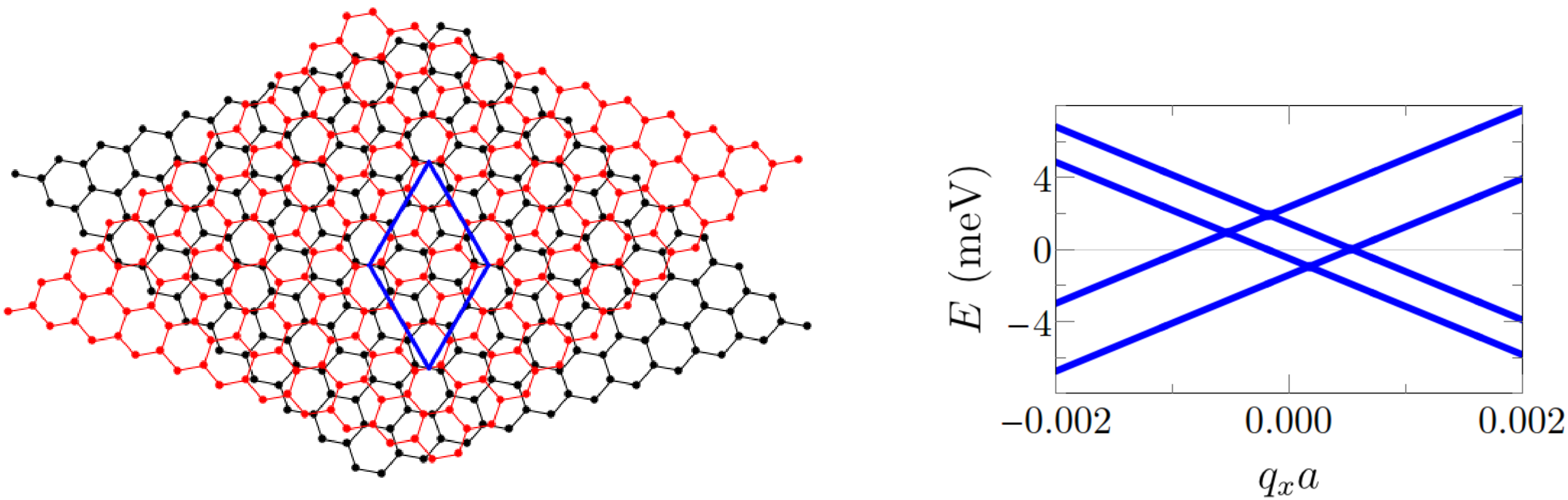

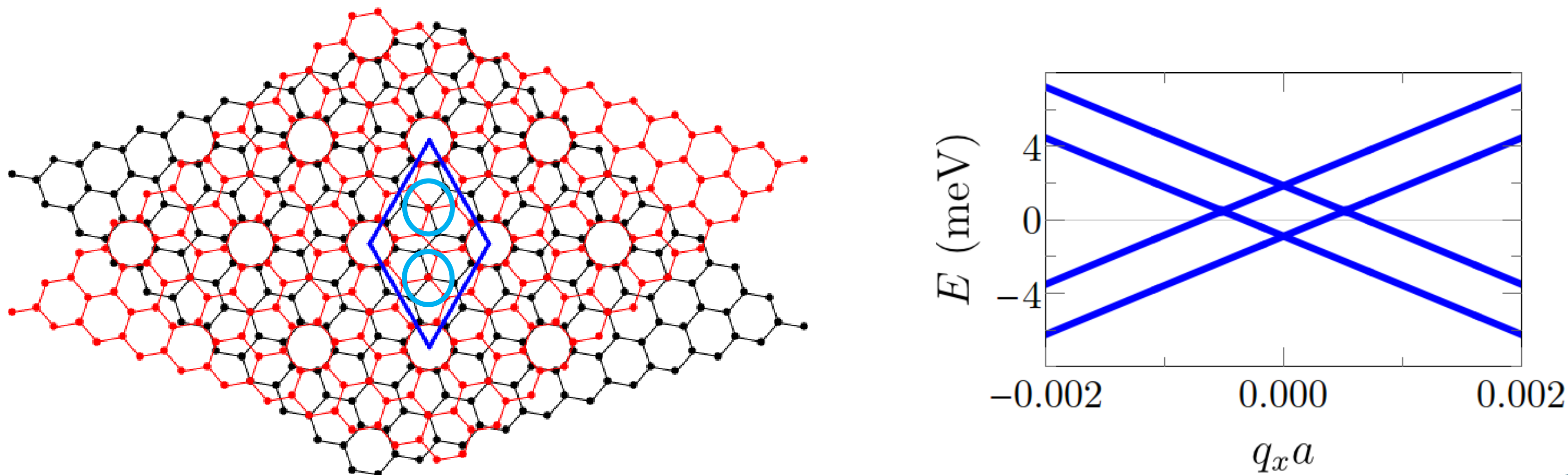

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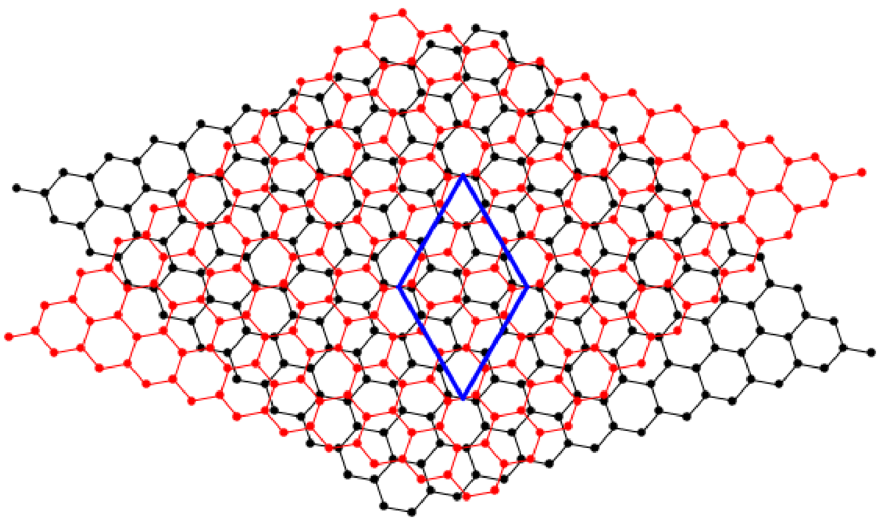

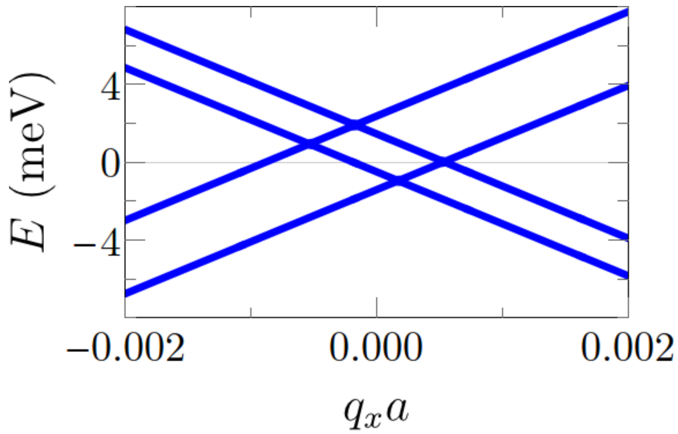

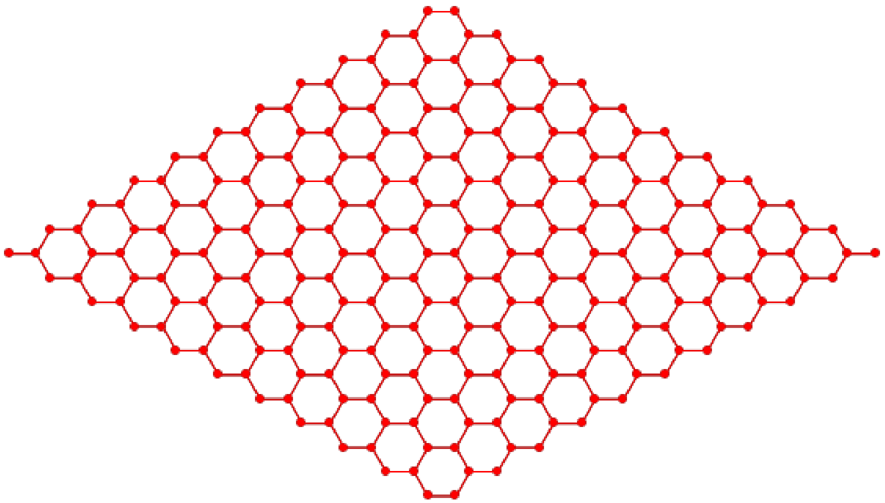

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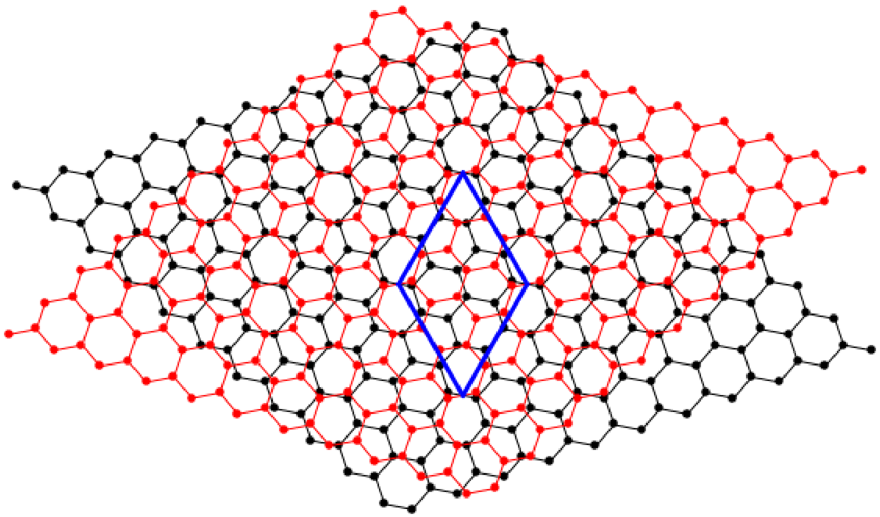

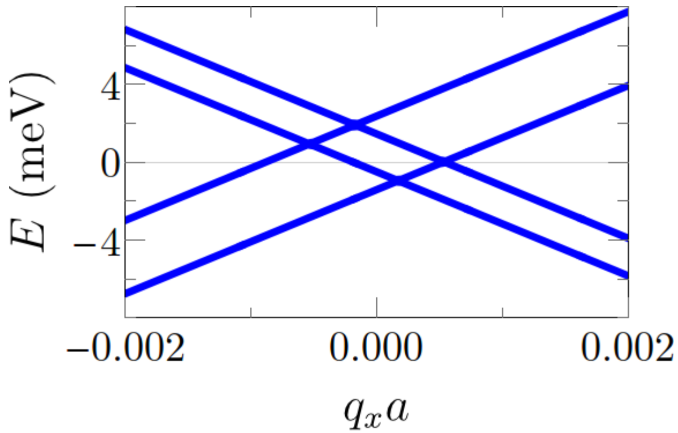

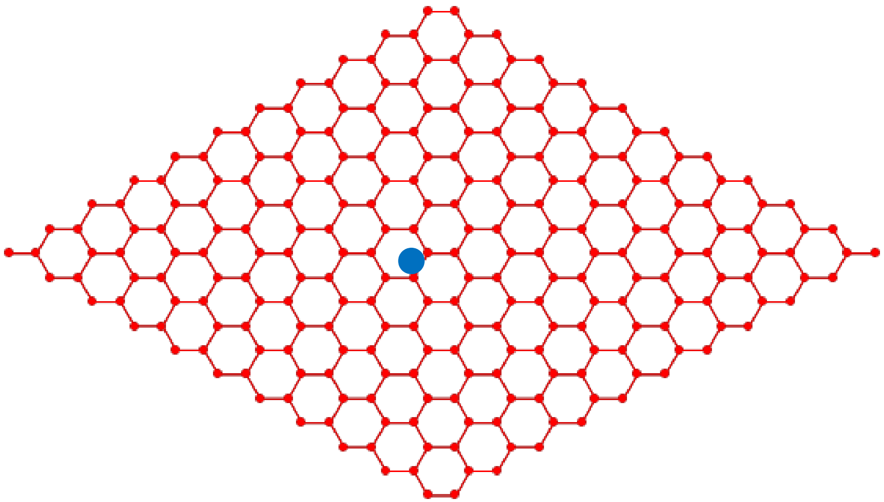

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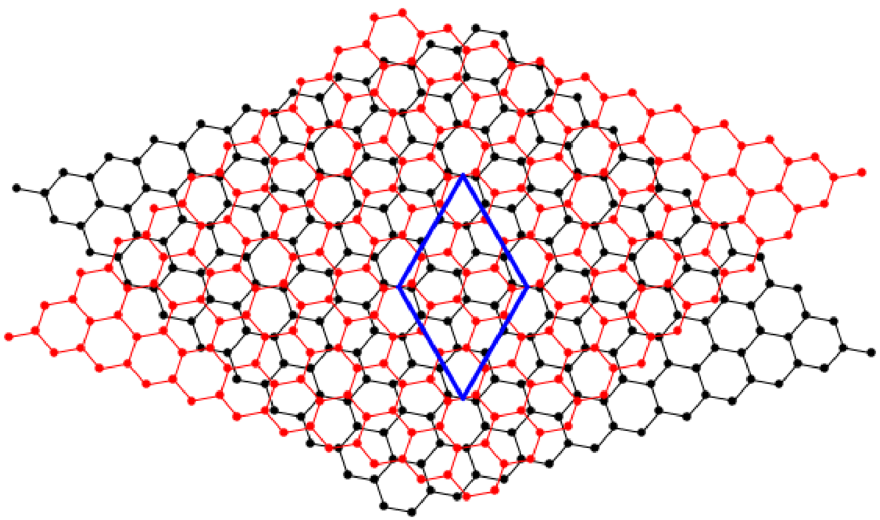

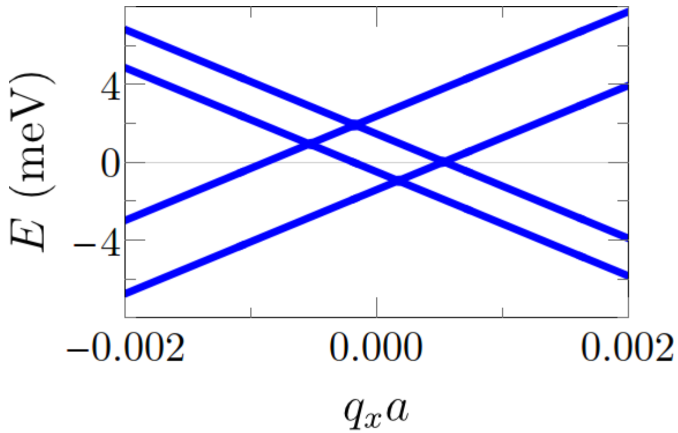

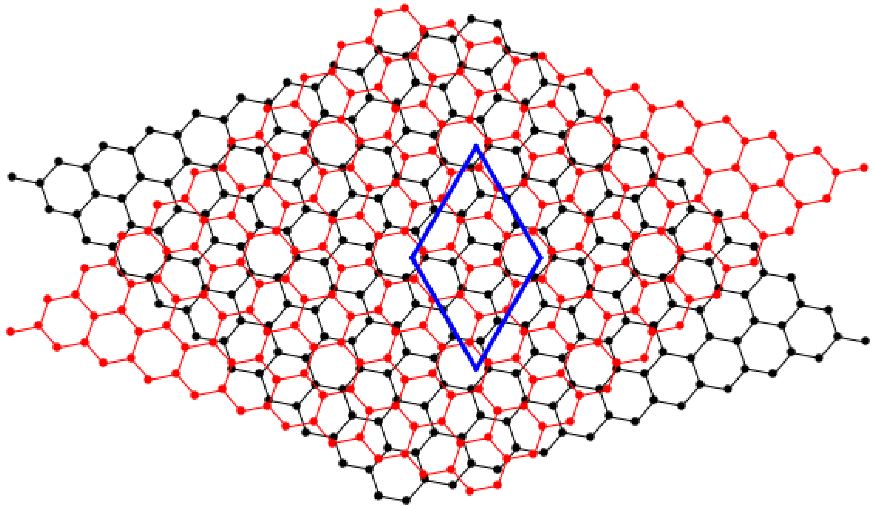

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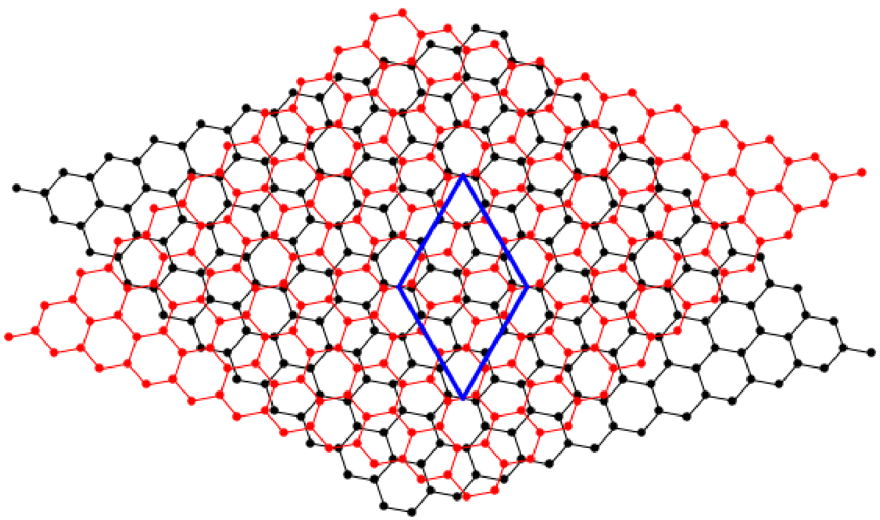

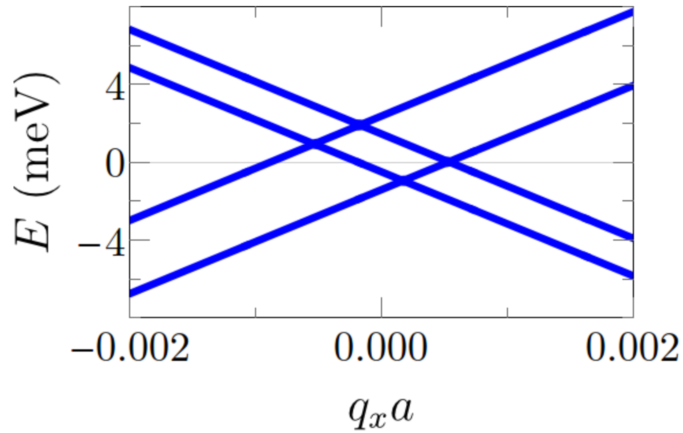

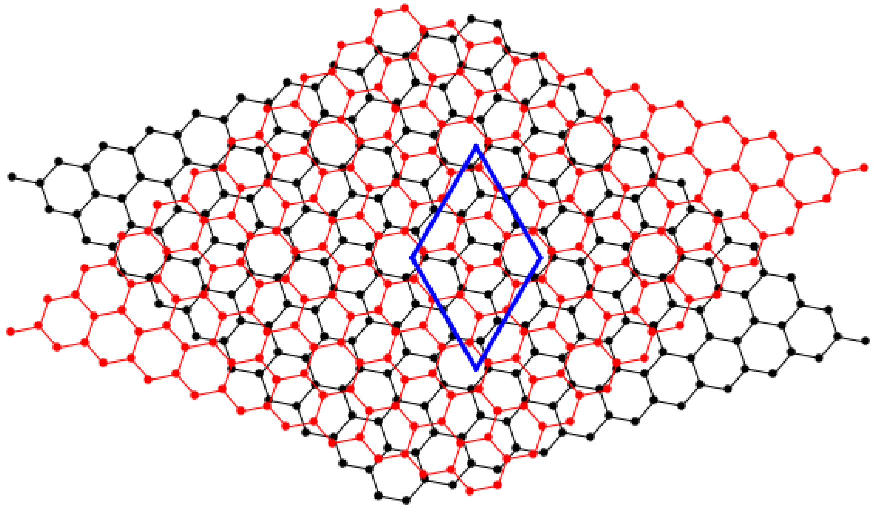

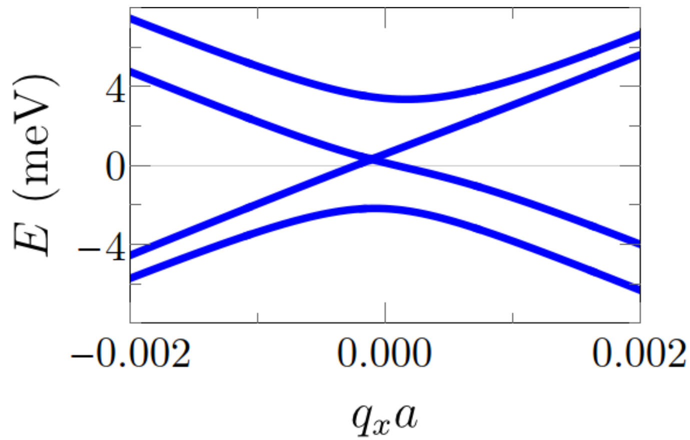

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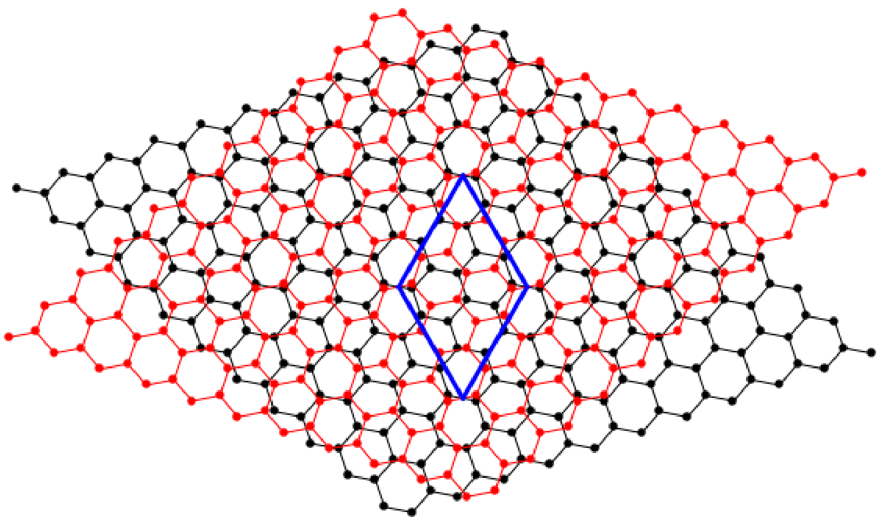

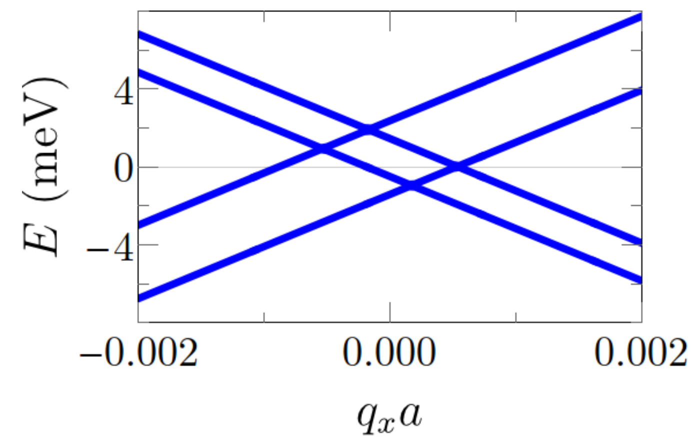

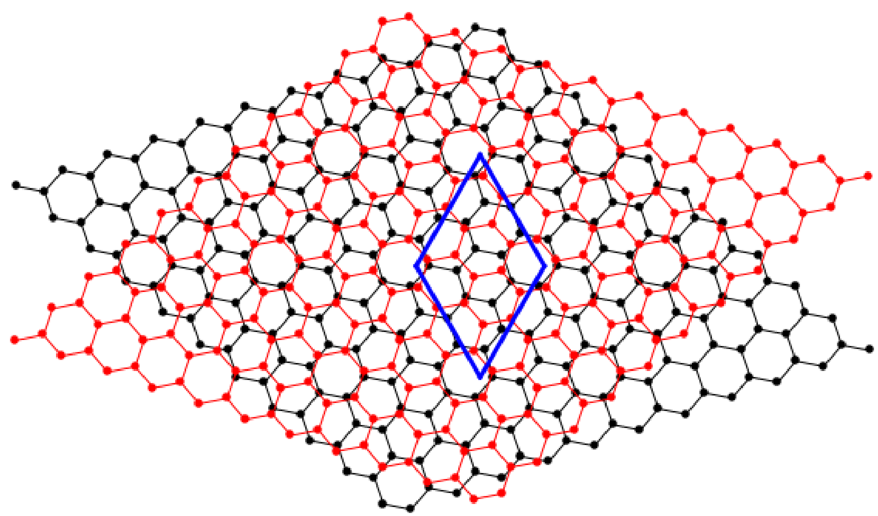

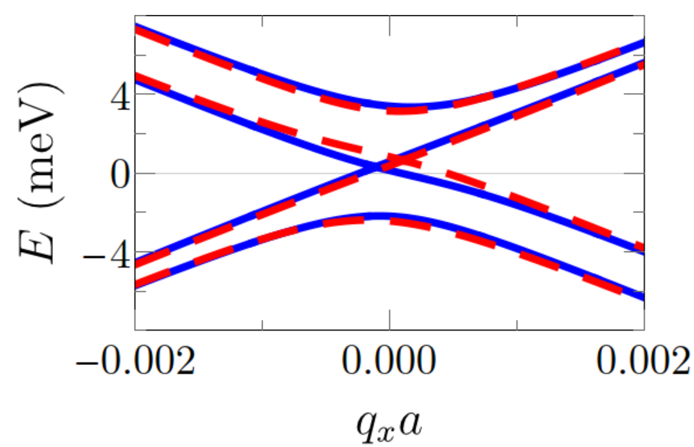

Triaxial strain

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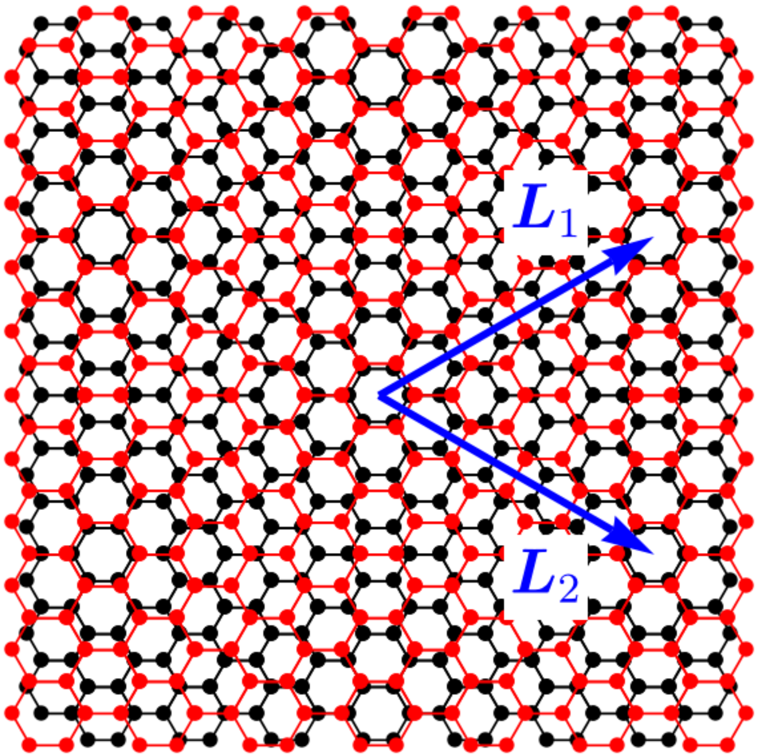

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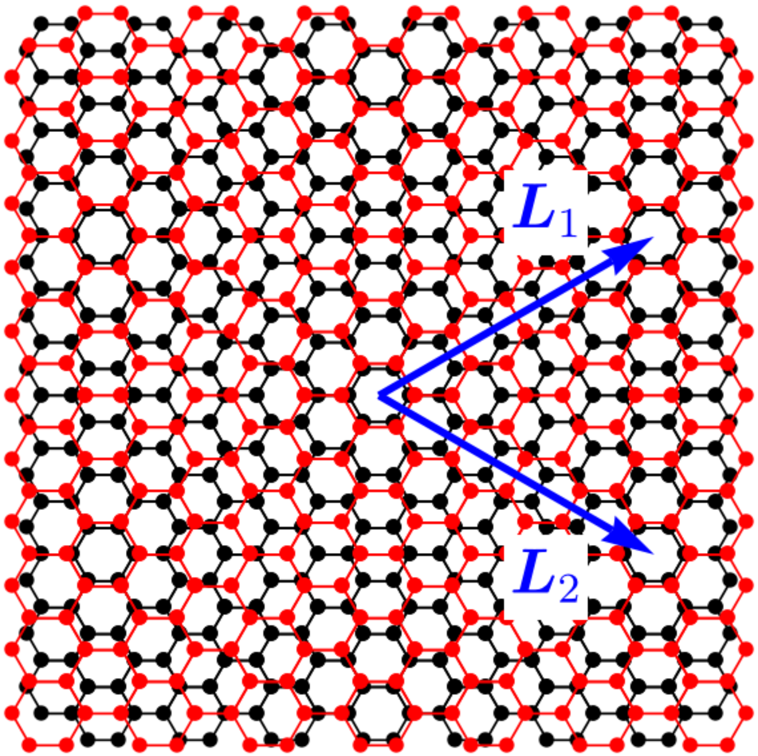

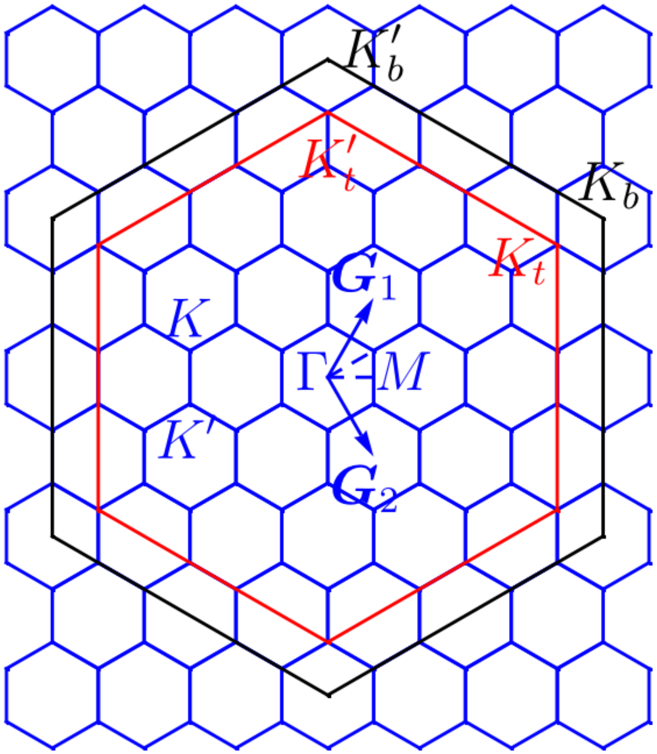

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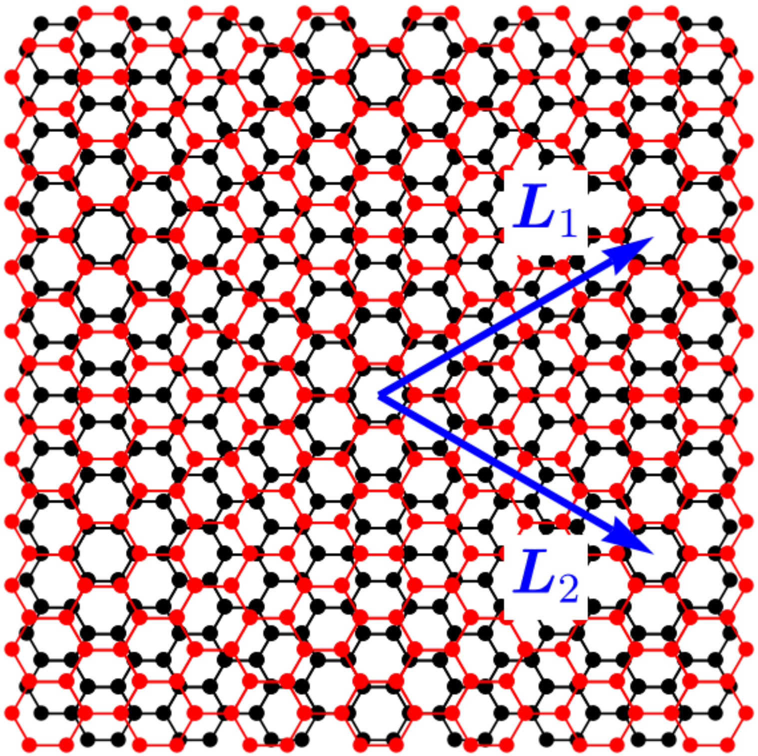

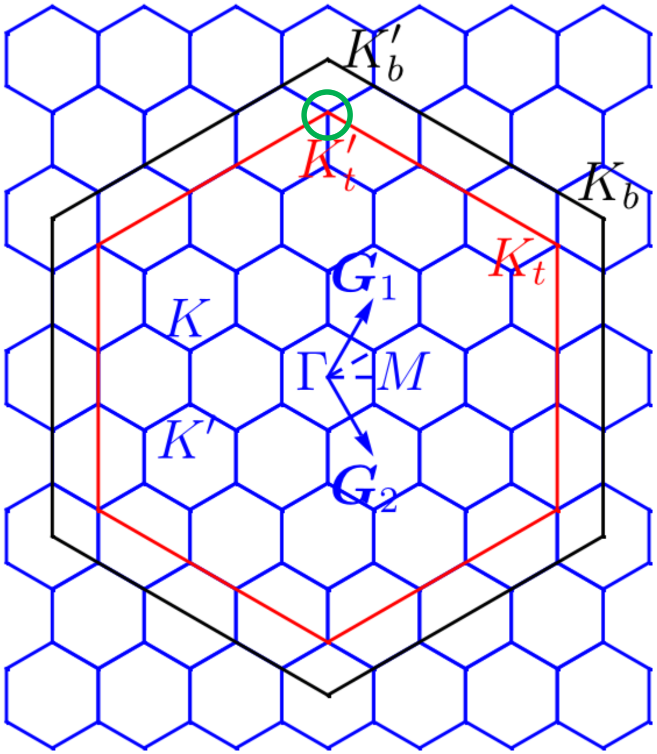

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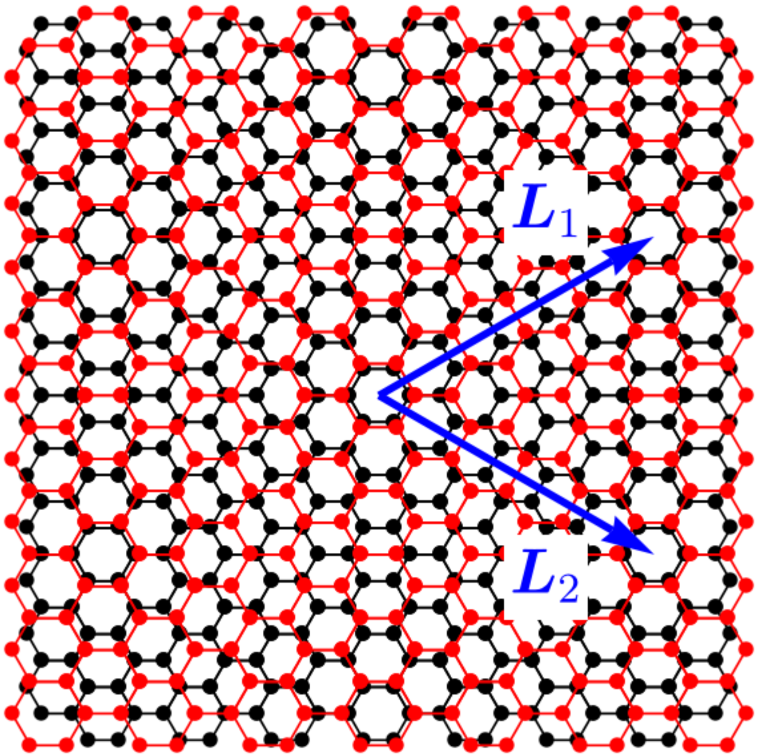

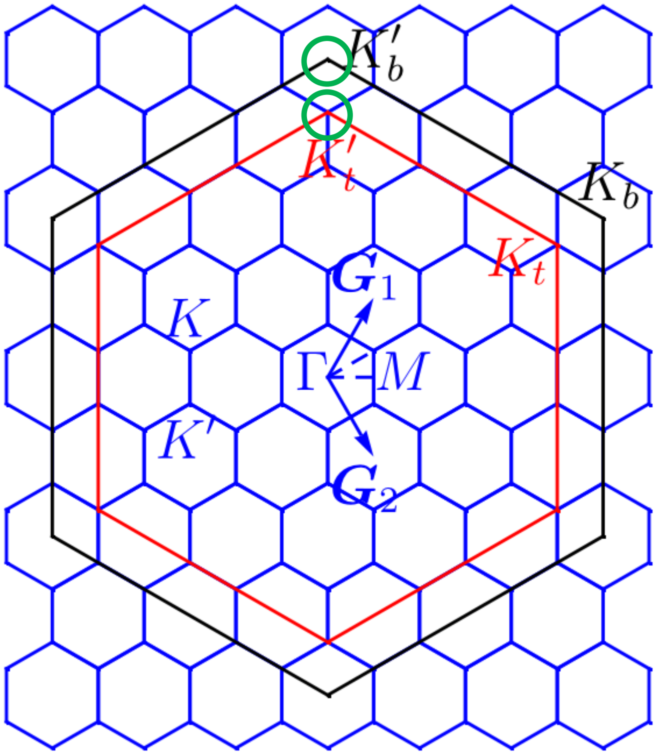

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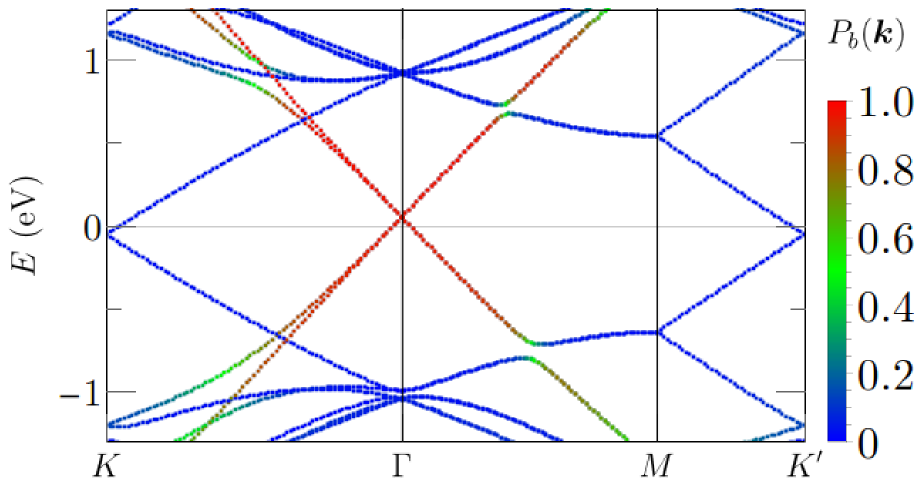
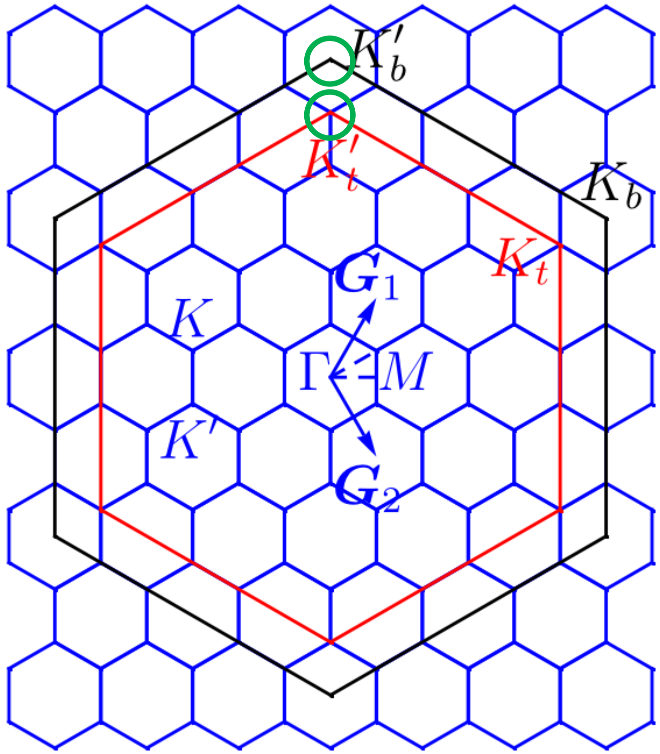
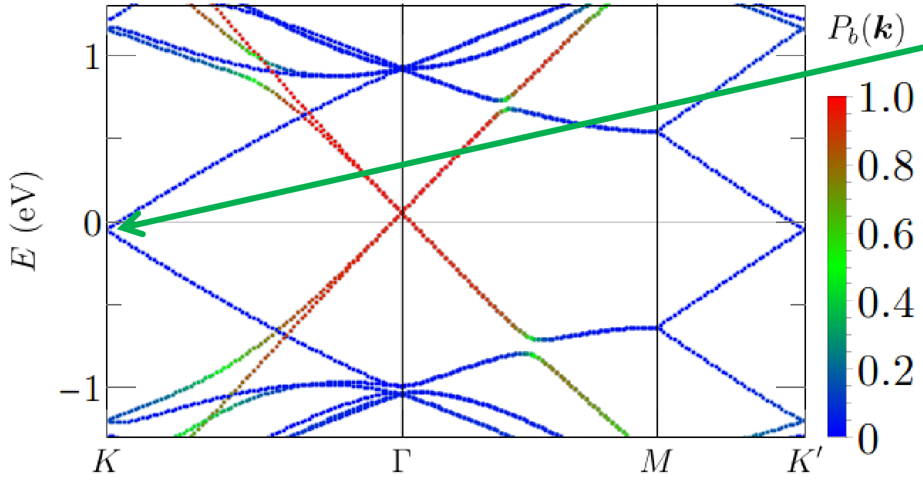
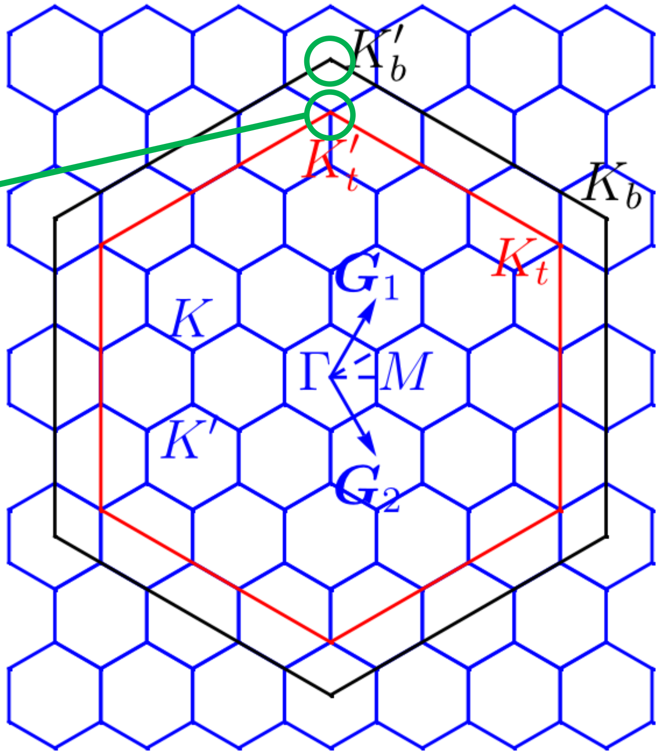


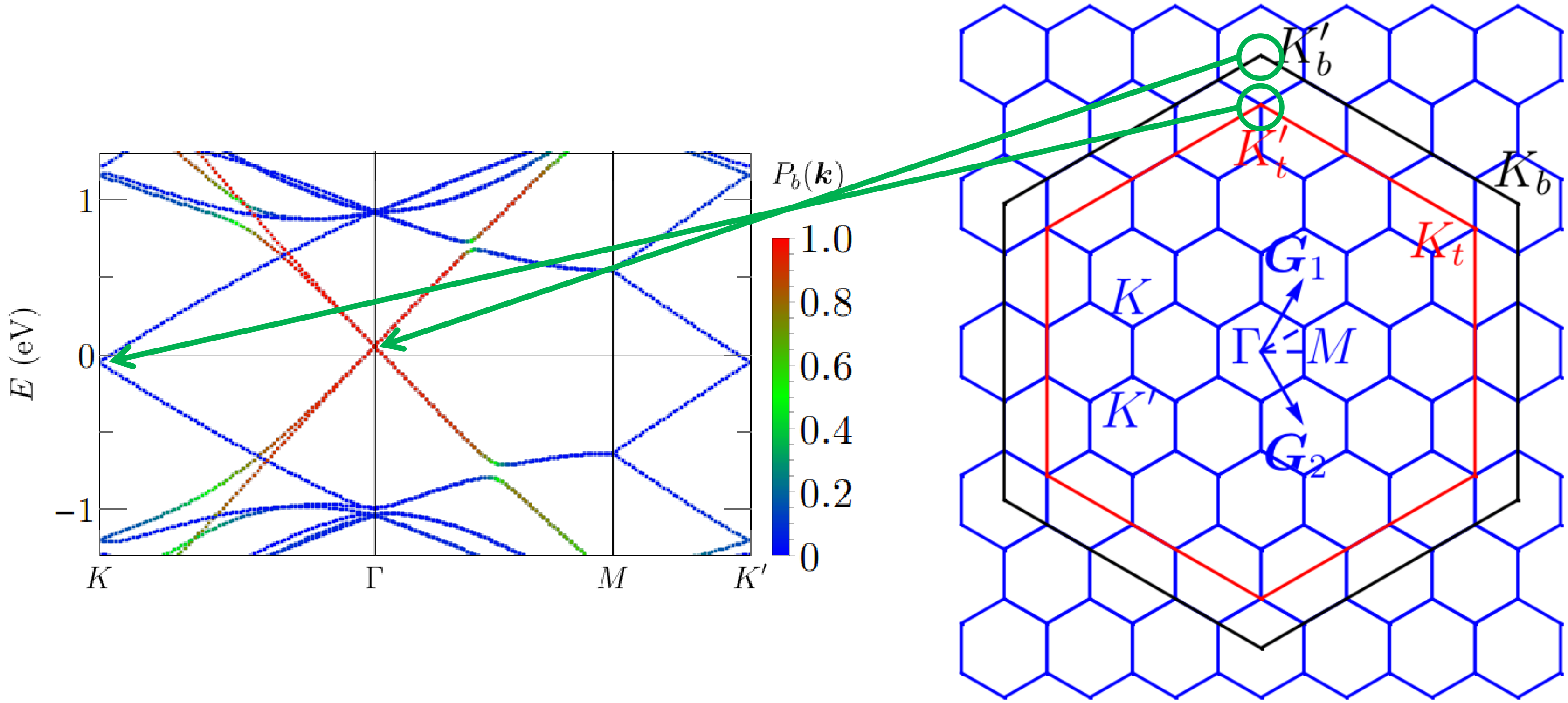


Triaxial strain

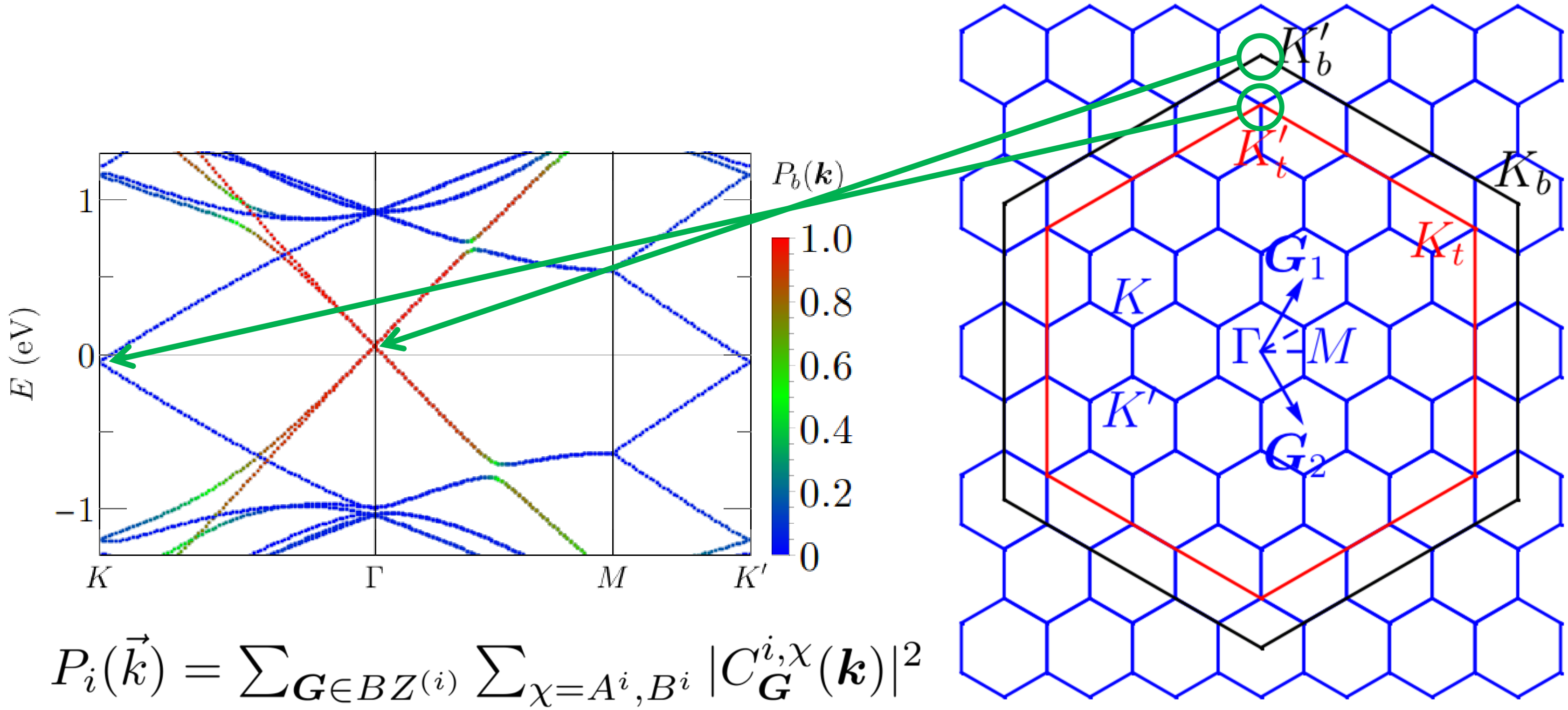




Triaxial strain

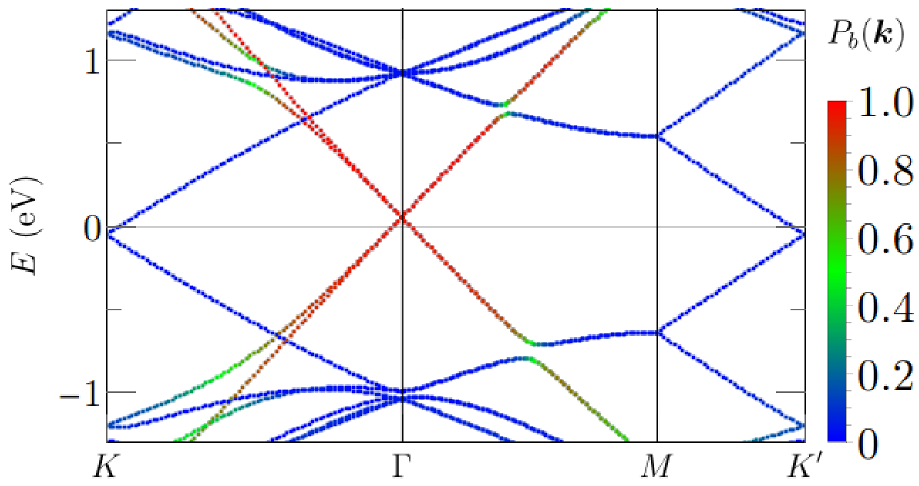


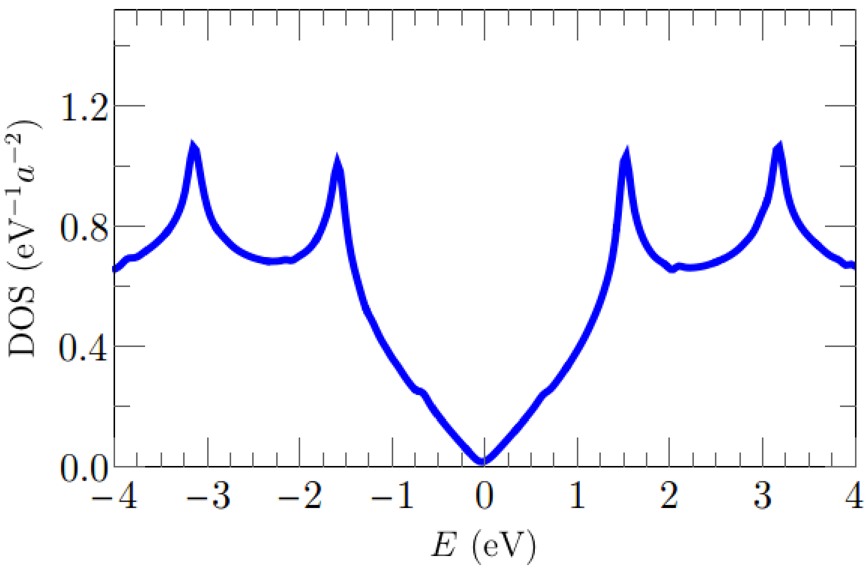
Triaxial strain



$$P_i(\vec{k}) = \sum_{\boldsymbol{G}\in BZ^{(i)}} \sum_{\chi=A^i,B^i} |C_{\boldsymbol{G}}^{i,\chi}(\boldsymbol{k})|^2$$

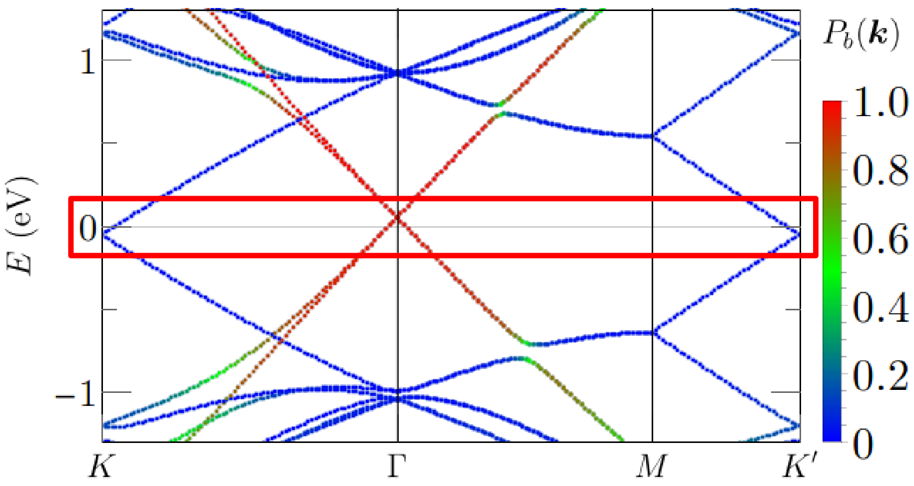
Triaxial strain

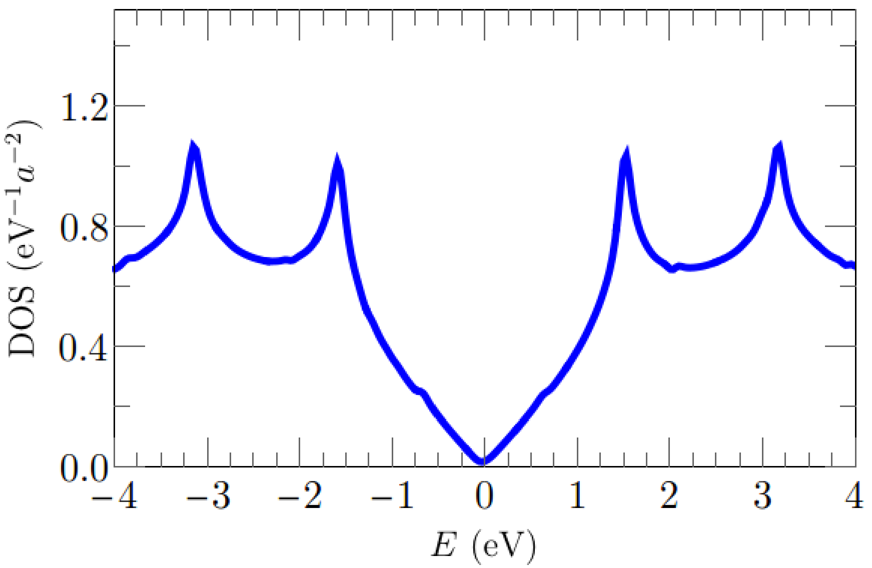




$$P_i(\vec{k}) = \sum_{\boldsymbol{G}\in BZ^{(i)}} \sum_{\chi=A^i,B^i} |C^{i,\chi}_{\boldsymbol{G}}(\boldsymbol{k})|^2$$

Triaxial strain





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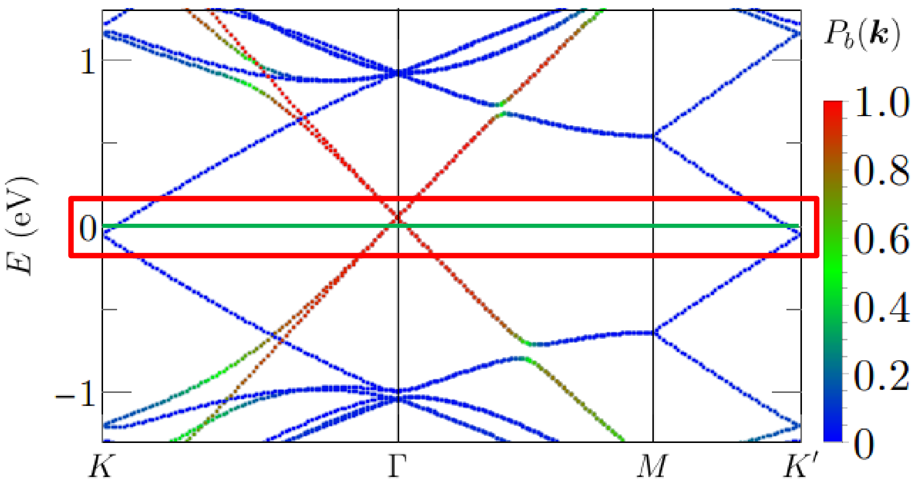
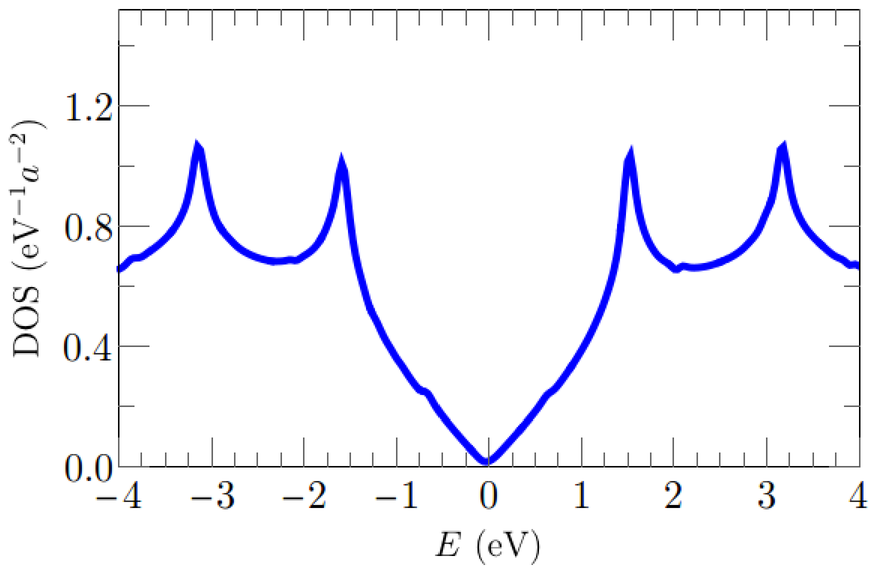
Triaxial strain





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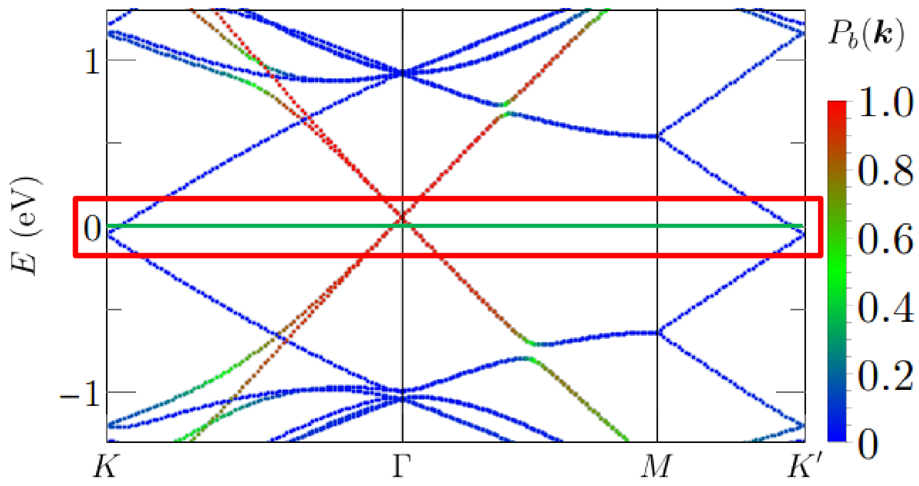
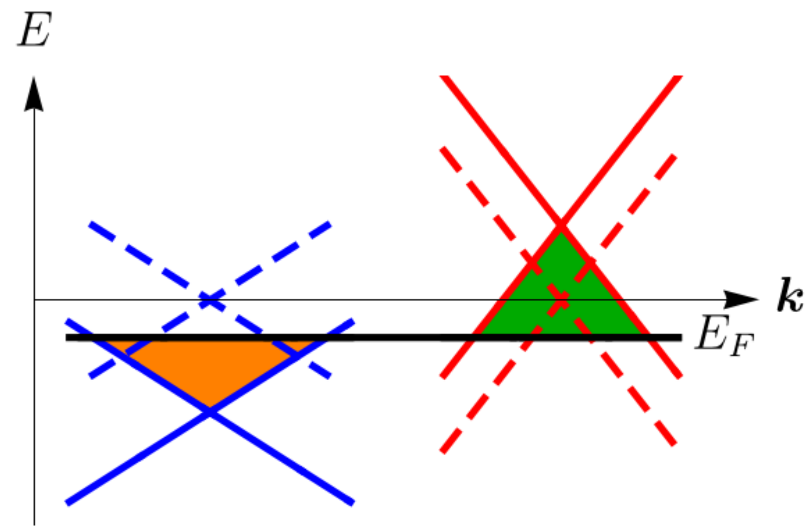
Triaxial strain





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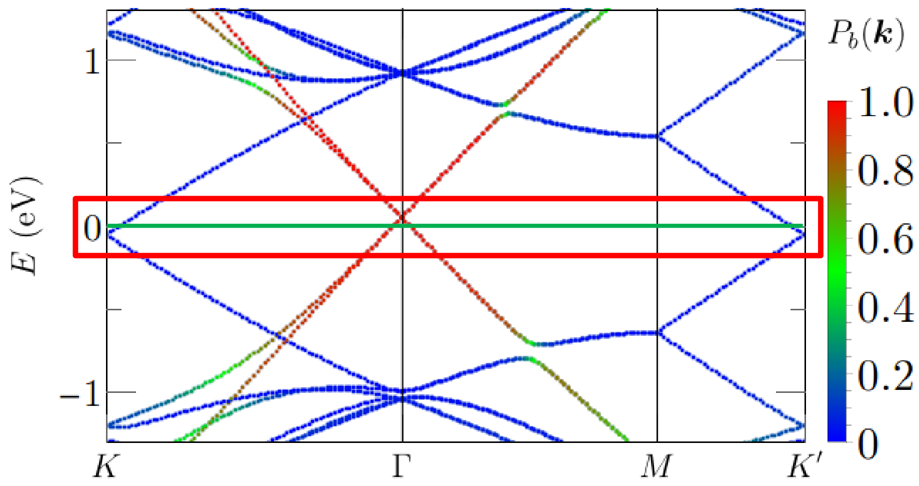
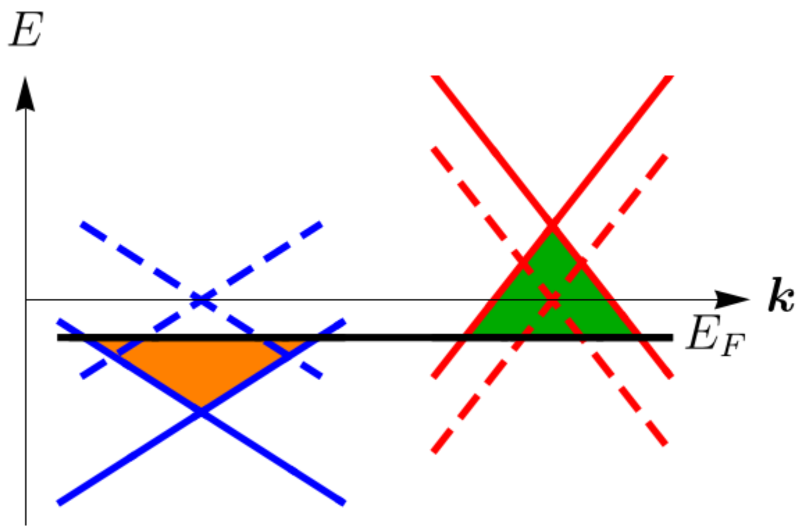
Triaxial strain

Piezoelectric effect!



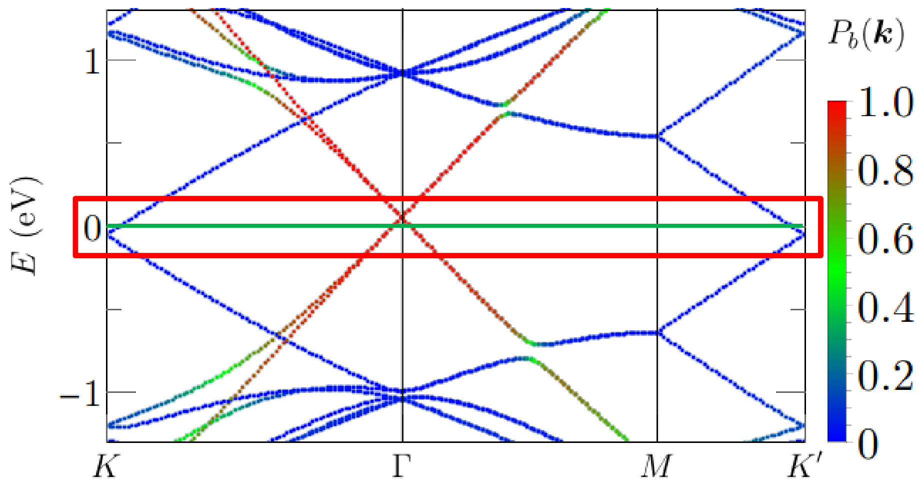


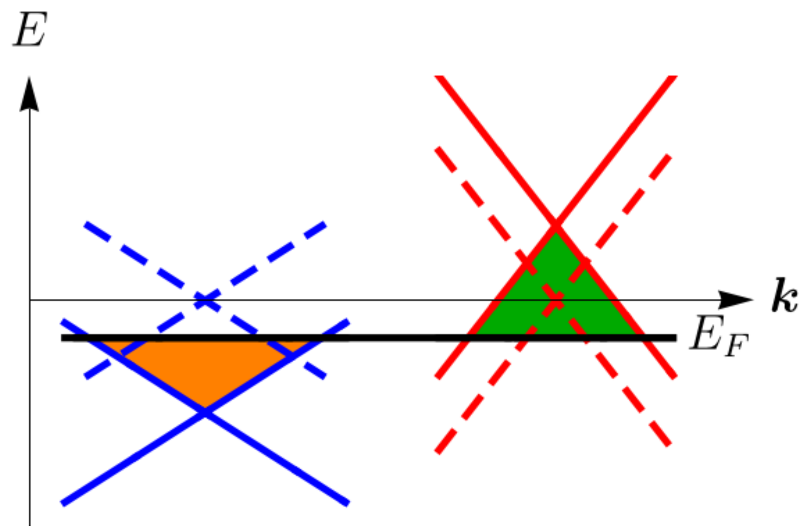
$$P_i(\vec{k}) = \sum_{\boldsymbol{G}\in BZ^{(i)}} \sum_{\chi=A^i,B^i} |C_{\boldsymbol{G}}^{i,\chi}(\boldsymbol{k})|^2$$

Triaxial strain

$$\Delta n = \frac{P_b(\boldsymbol{D}_b)+P_t(\boldsymbol{D}_t)-1}{\pi\hbar^2}\left(\frac{E_D^b-E_D^t}{v_F^b+v_F^t}\right)^2$$

Piezoelectric effect!





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Triaxial strain

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Triaxial strain

$$\Delta n = \frac{P_b(\boldsymbol{D}_b)+P_t(\boldsymbol{D}_t)-1}{\pi\hbar^2}\left(\frac{\boxed{E_D^b-E_D^t}}{v_F^b+v_F^t}\right)^2$$

Triaxial strain

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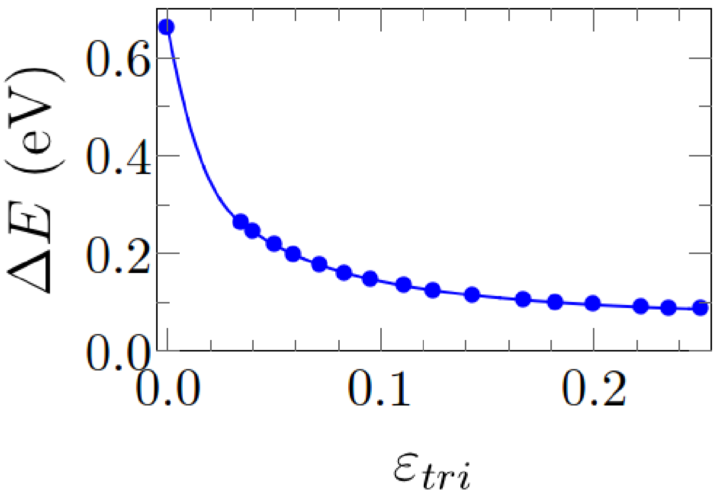
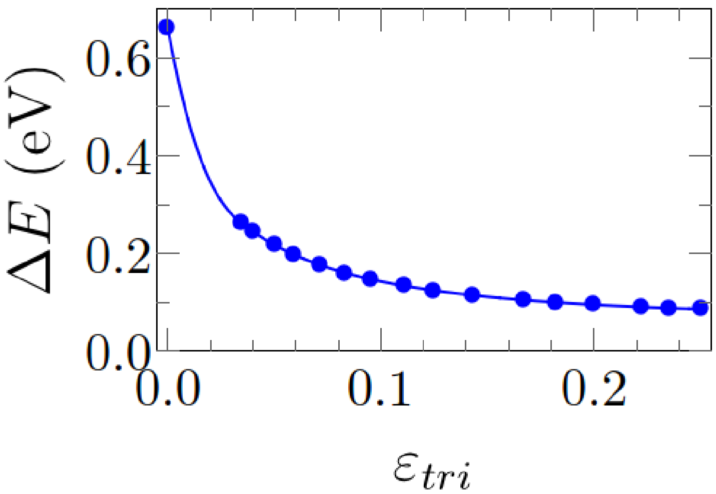


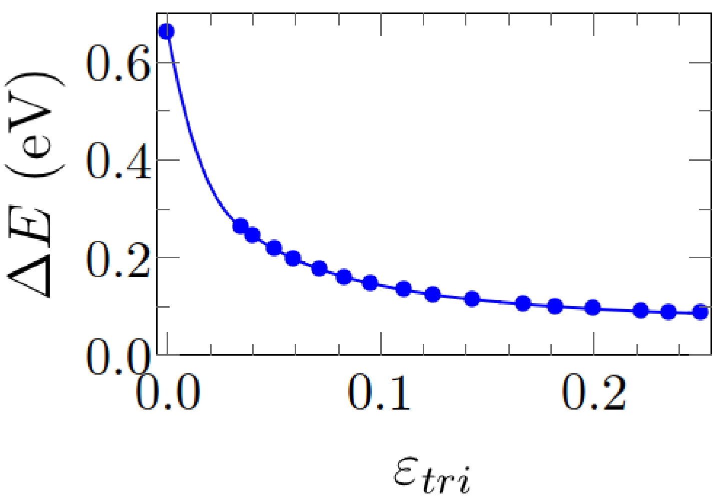
Triaxial strain

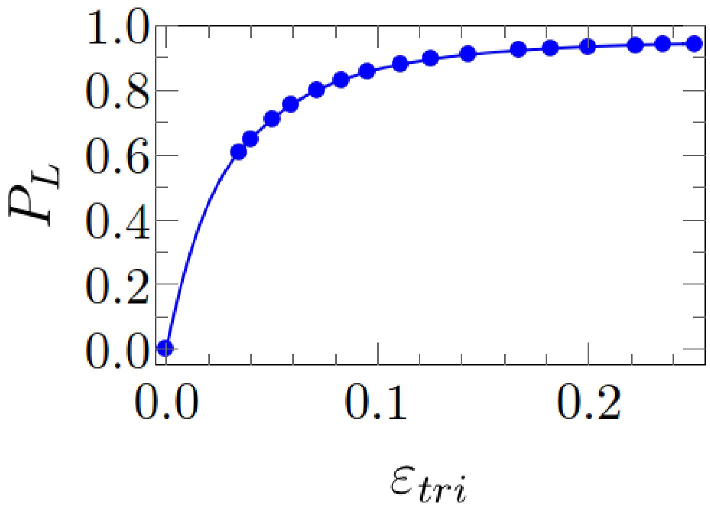
$$\Delta n = \frac{\boxed{P_b(\boldsymbol{D}_b)+P_t(\boldsymbol{D}_t)-1}}{\pi\hbar^2}\left(\frac{E_D^b-E_D^t}{v_F^b+v_F^t}\right)^2$$



Triaxial strain

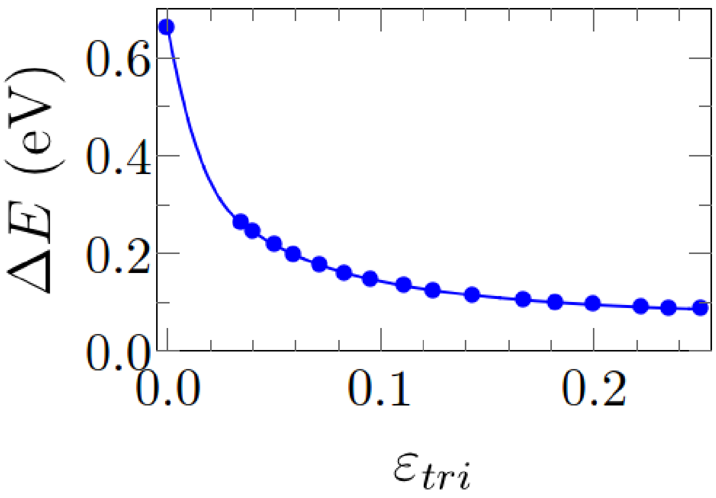
$$\Delta n = \frac{\boxed{P_b(\boldsymbol{D}_b)+P_t(\boldsymbol{D}_t)-1}}{\pi\hbar^2}\left(\frac{E_D^b-E_D^t}{v_F^b+v_F^t}\right)^2$$

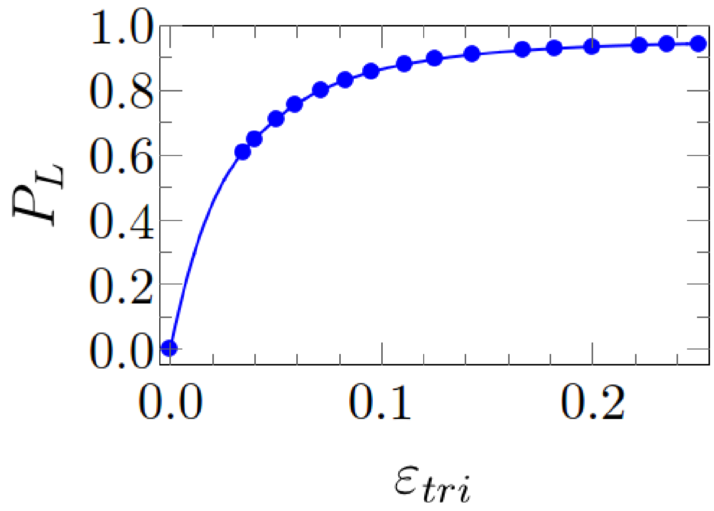


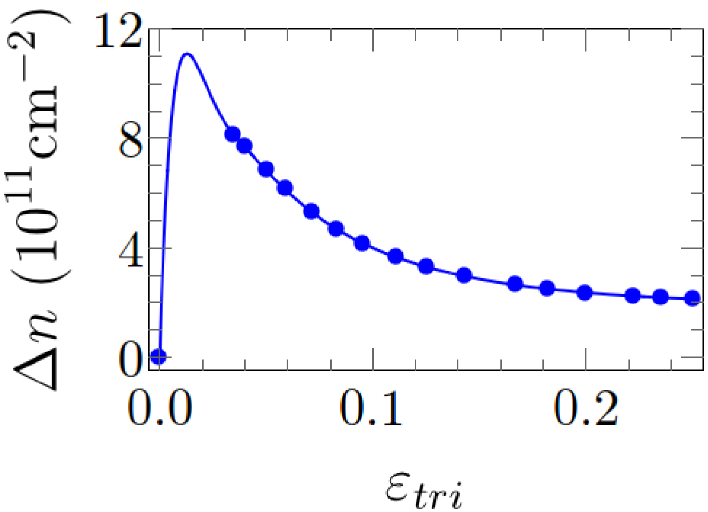


Triaxial strain

$$\Delta n = \frac{P_b(\boldsymbol{D}_b)+P_t(\boldsymbol{D}_t)-1}{\pi\hbar^2}\left(\frac{E_D^b-E_D^t}{v_F^b+v_F^t}\right)^2$$







Triaxial strain

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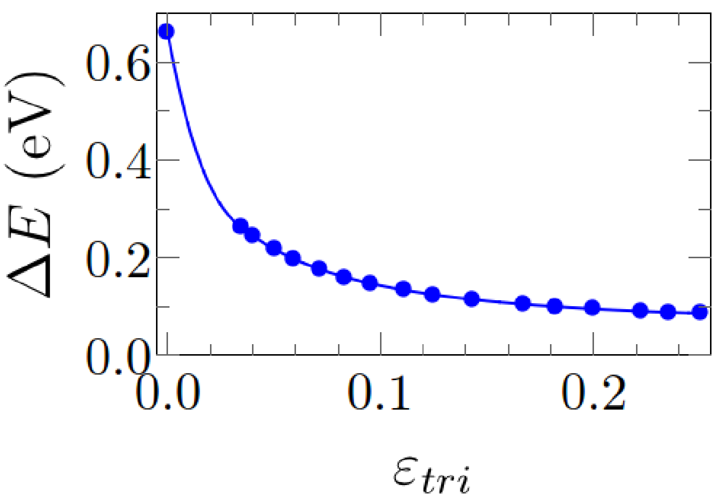
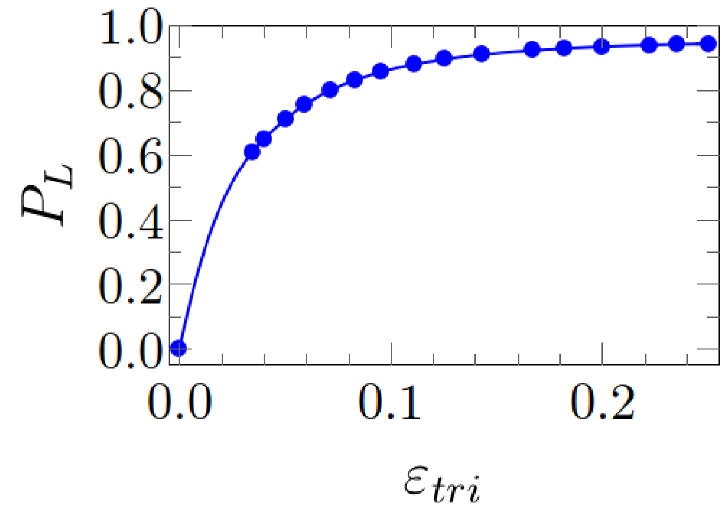
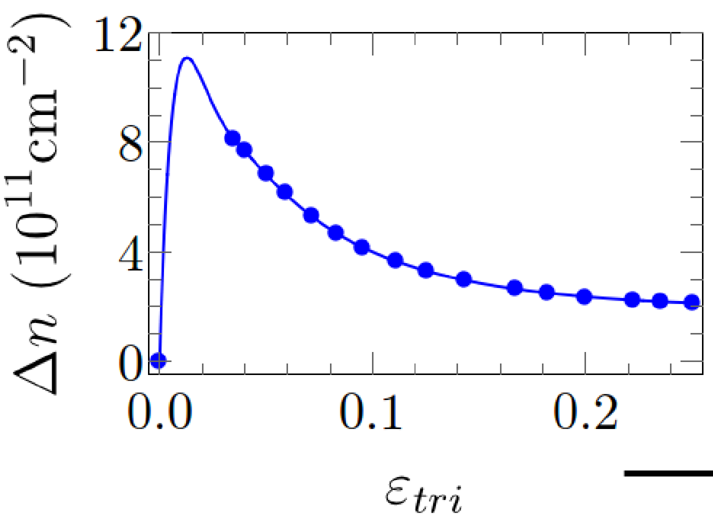
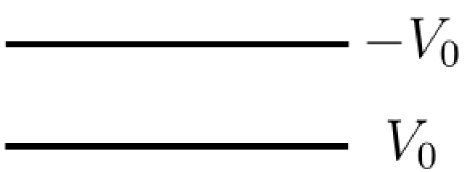


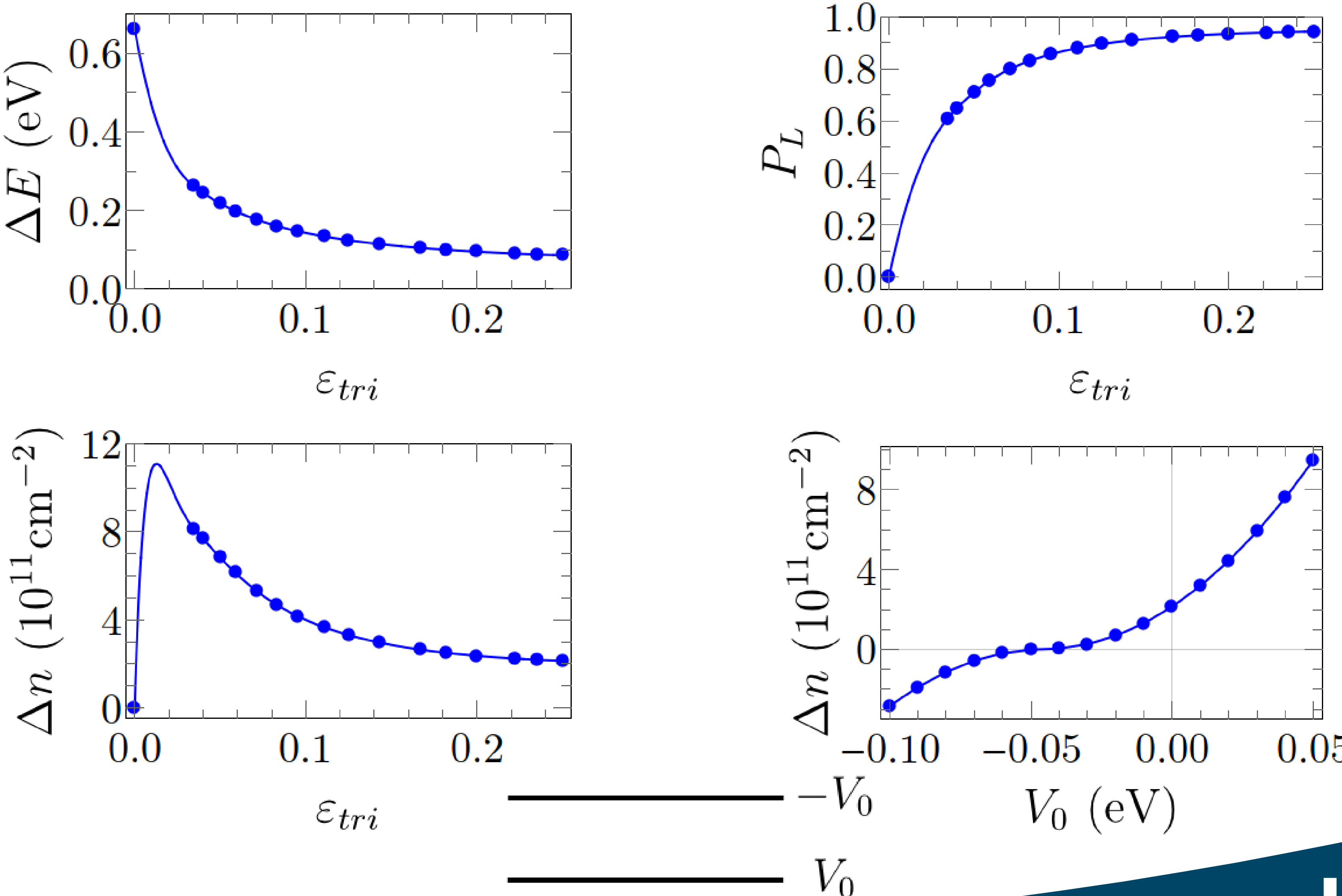






Triaxial strain

$$\Delta n = \frac{P_b(\boldsymbol{D}_b)+P_t(\boldsymbol{D}_t)-1}{\pi\hbar^2}\left(\frac{E_D^b-E_D^t}{v_F^b+v_F^t}\right)^2$$



Uniaxial strain

Uniaxial strain

Armchair

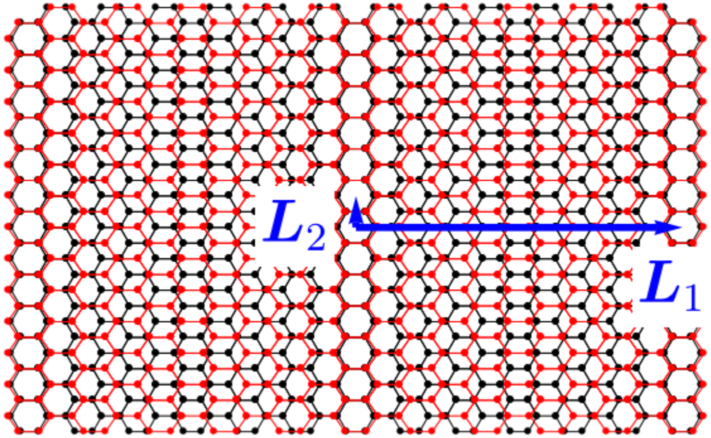
Uniaxial strain

Armchair

Zigzag

Uniaxial strain

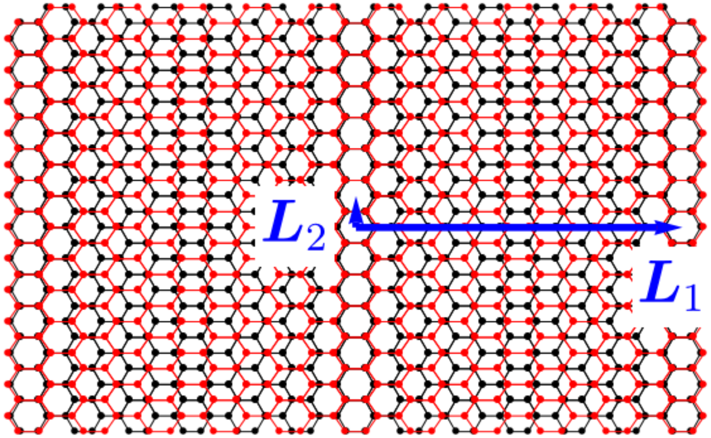
Armchair



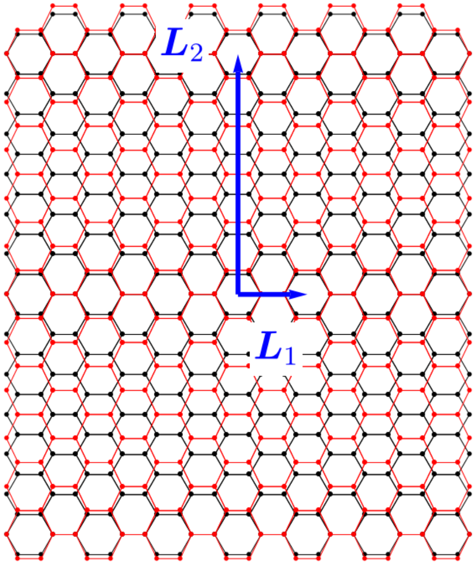
Zigzag

Uniaxial strain

Armchair

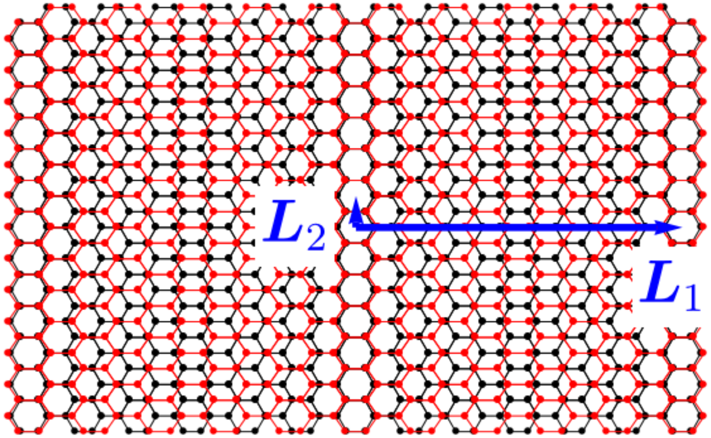


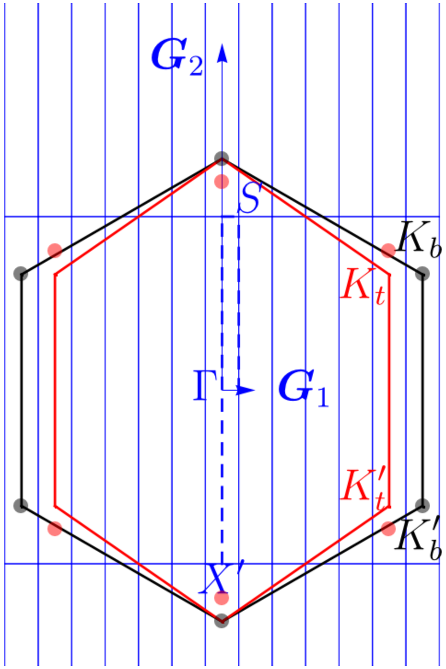
Zigzag



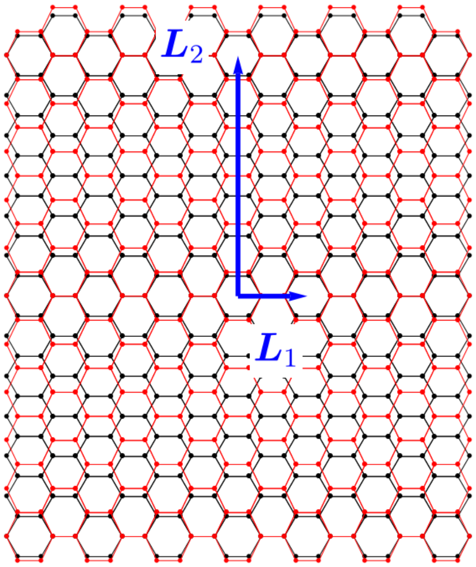
Uniaxial strain

Armchair



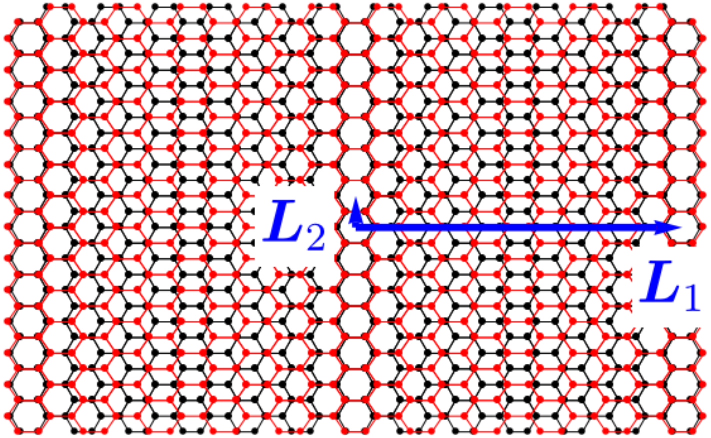


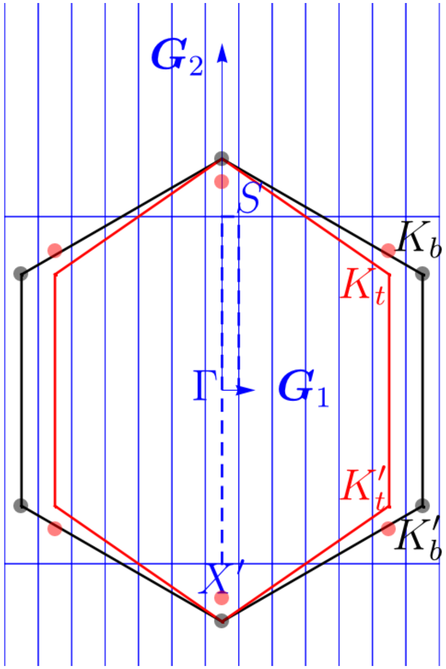
Zigzag



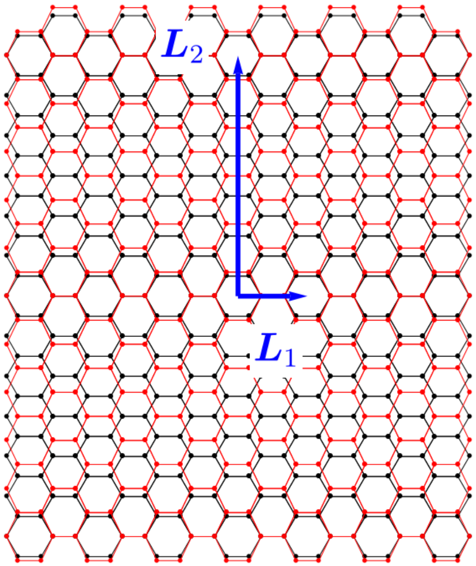
Uniaxial strain

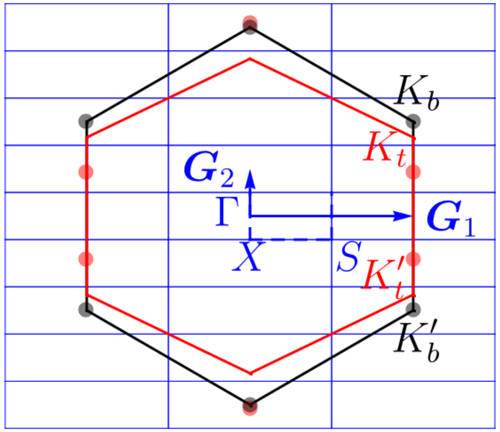
Armchair





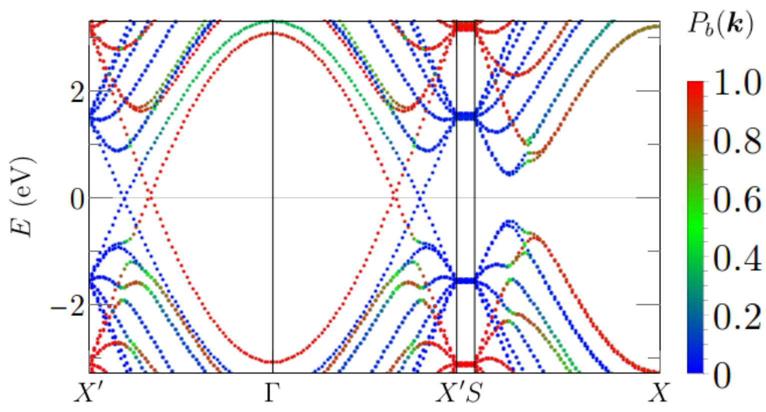
Zigzag

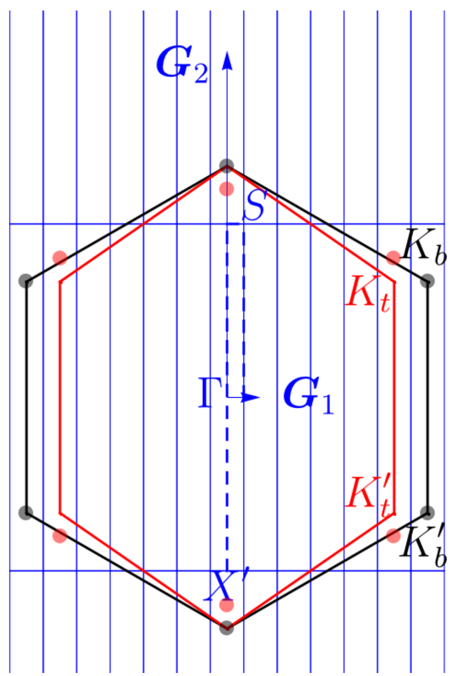




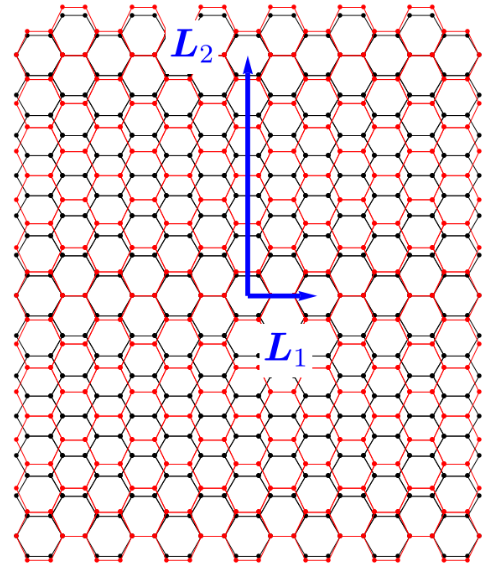
Uniaxial strain

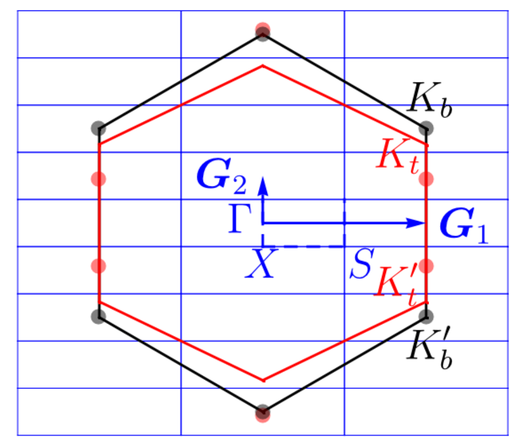
Armchair





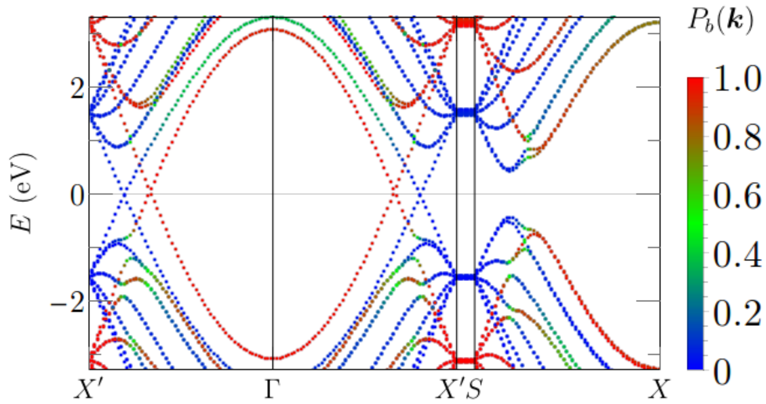
Zigzag

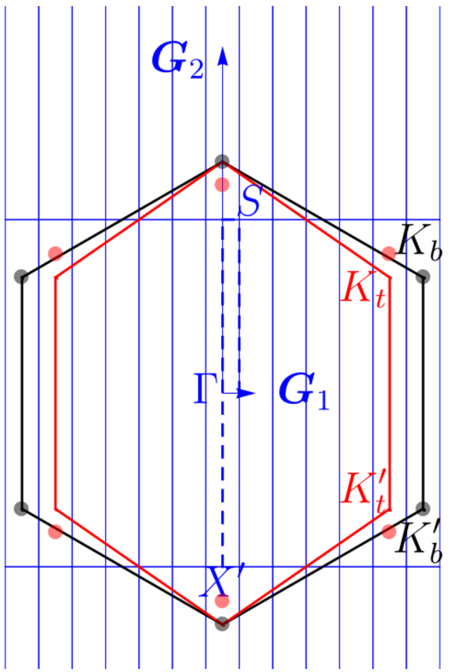




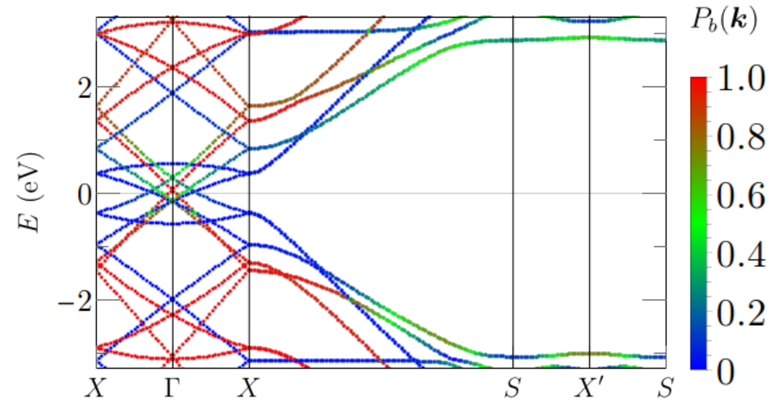
Uniaxial strain

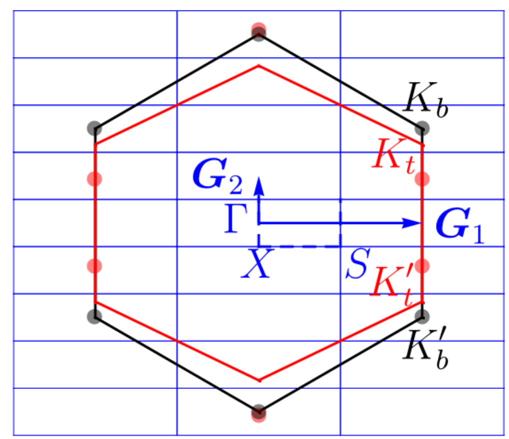
Armchair





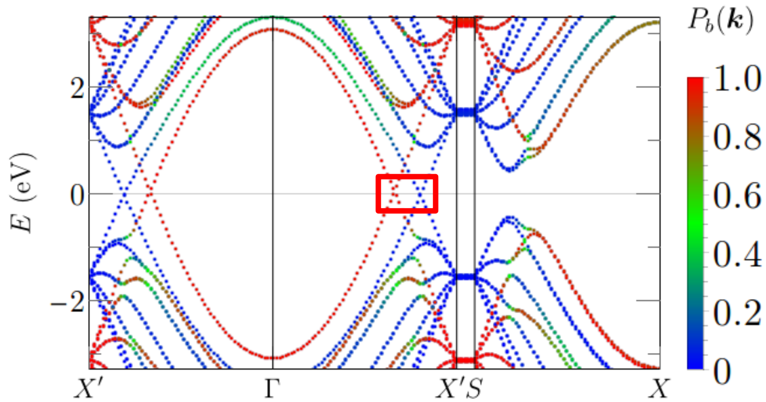
Zigzag

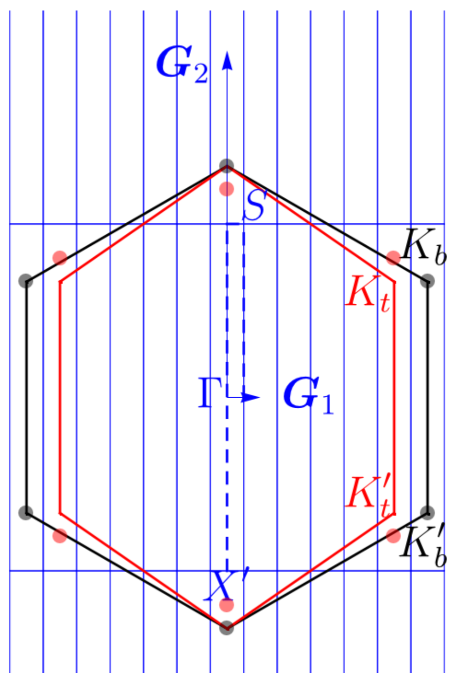




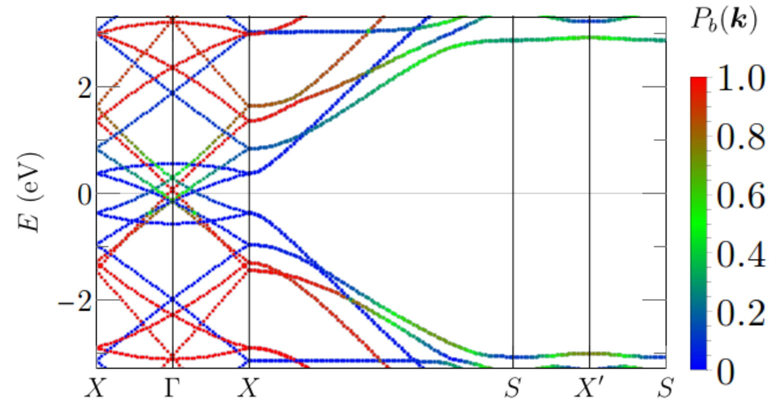
Uniaxial strain

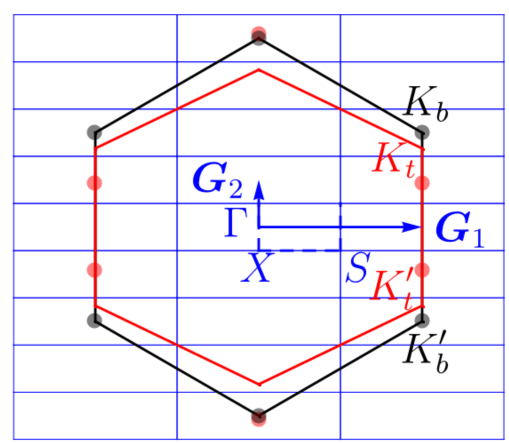
Armchair





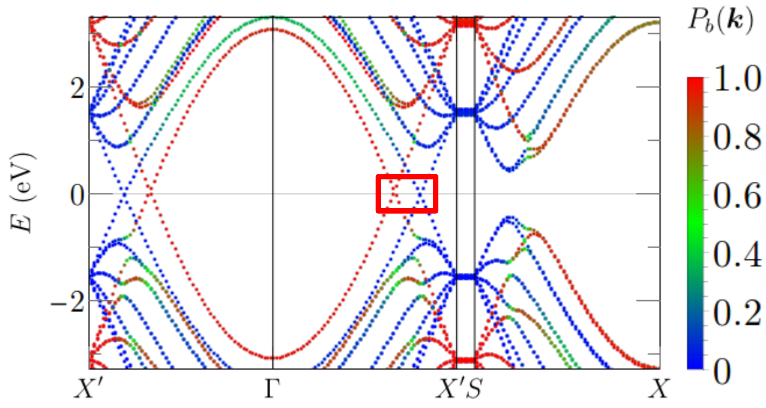
Zigzag



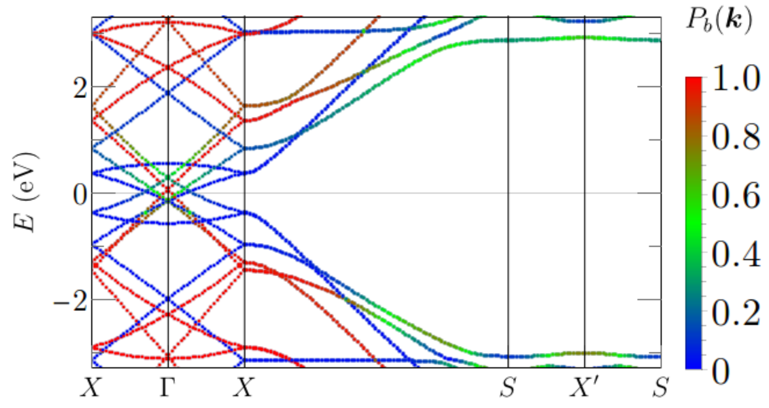


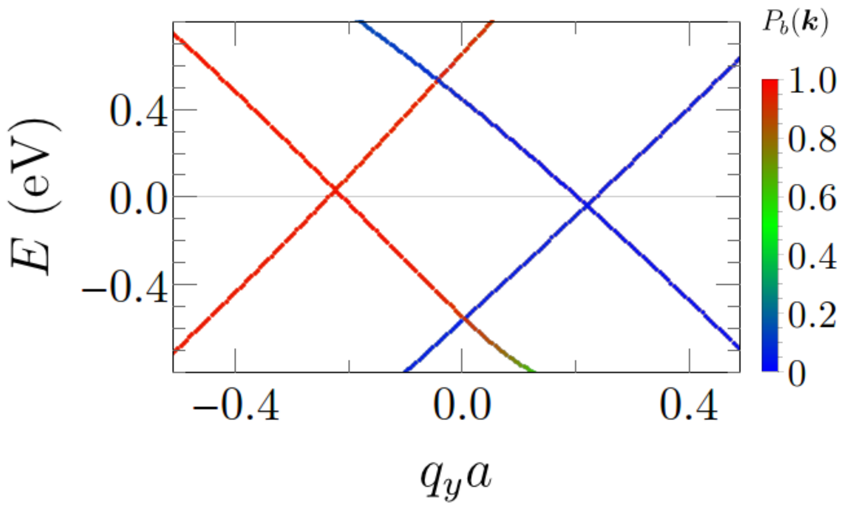
Uniaxial strain

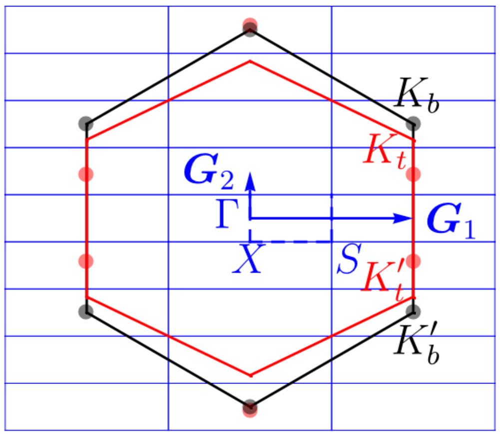
Armchair



Zigzag

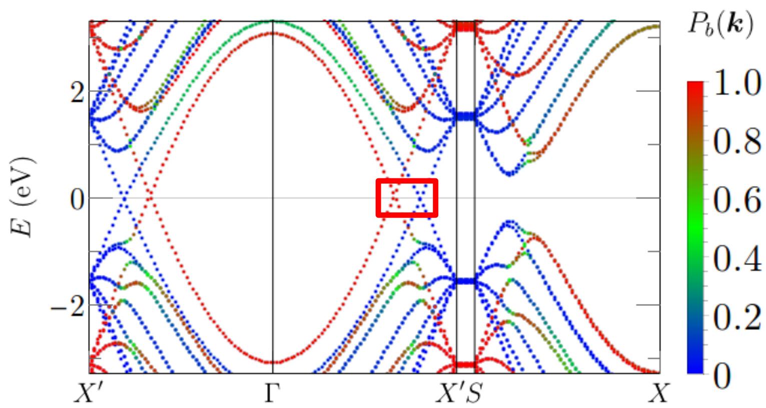




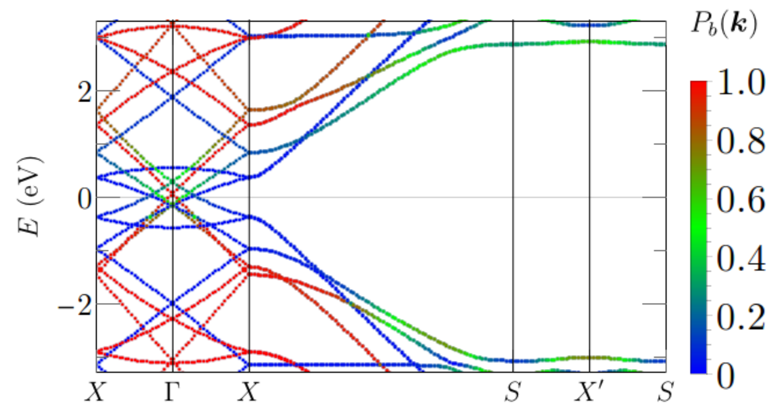


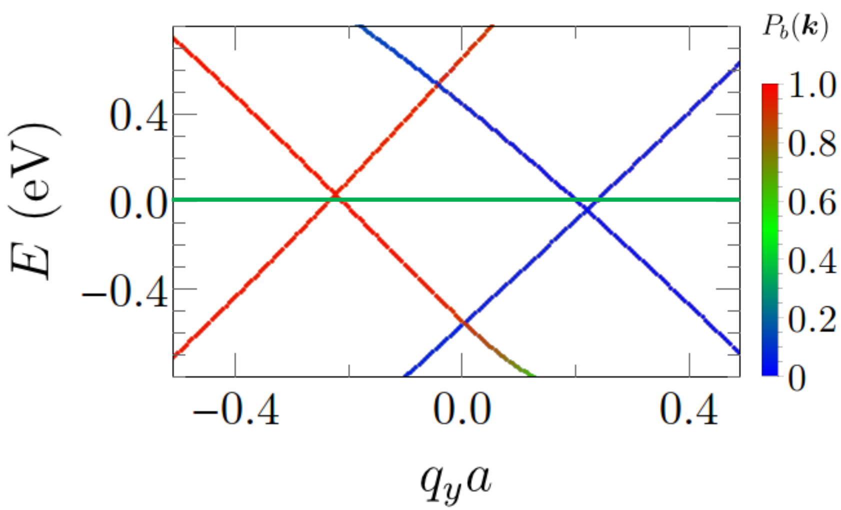
Uniaxial strain

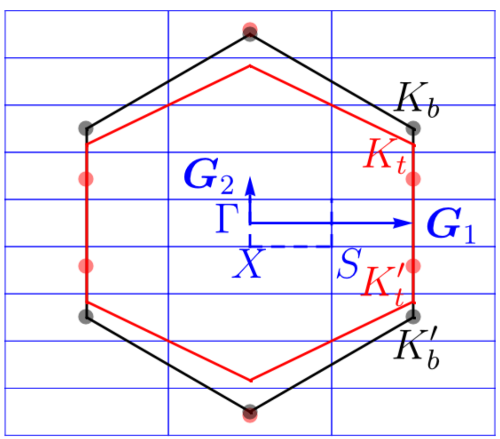
Armchair



Zigzag

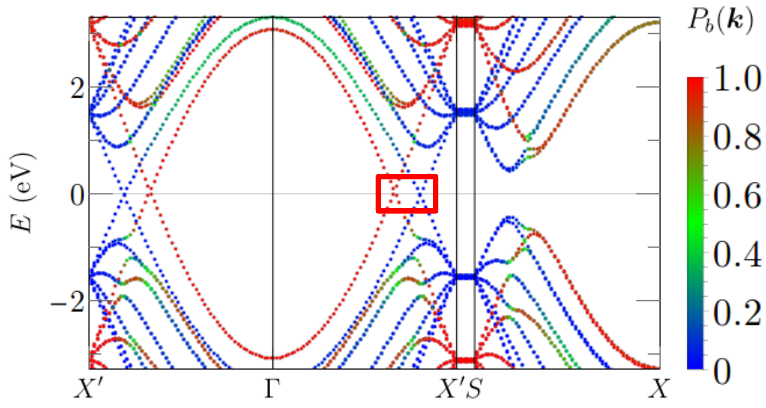




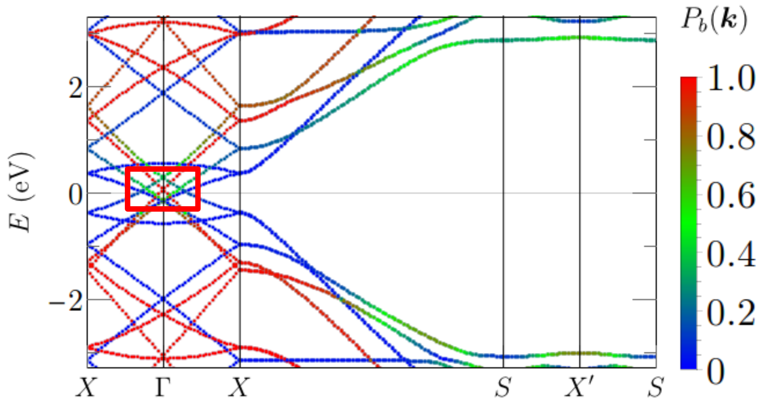


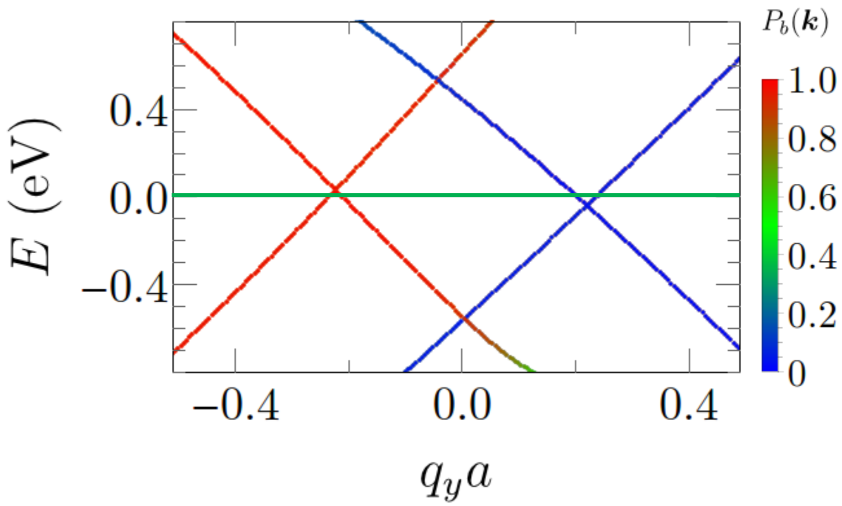
Uniaxial strain

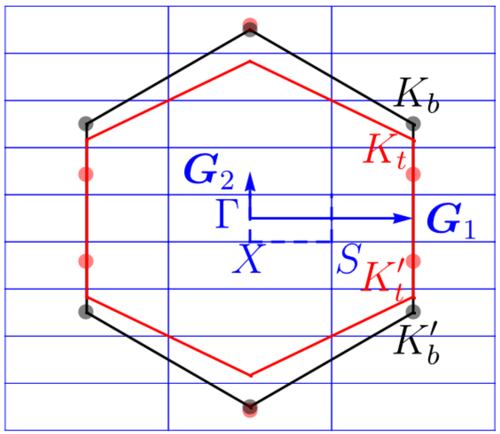
Armchair



Zigzag







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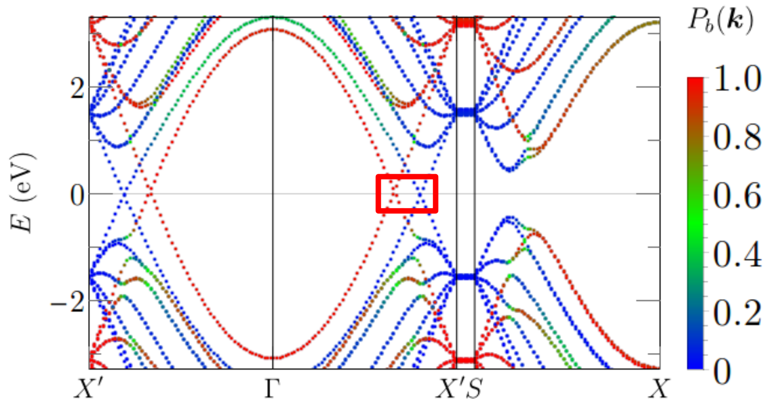
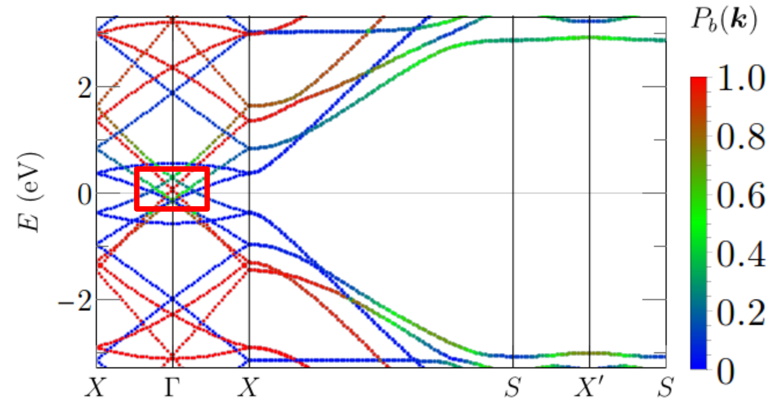
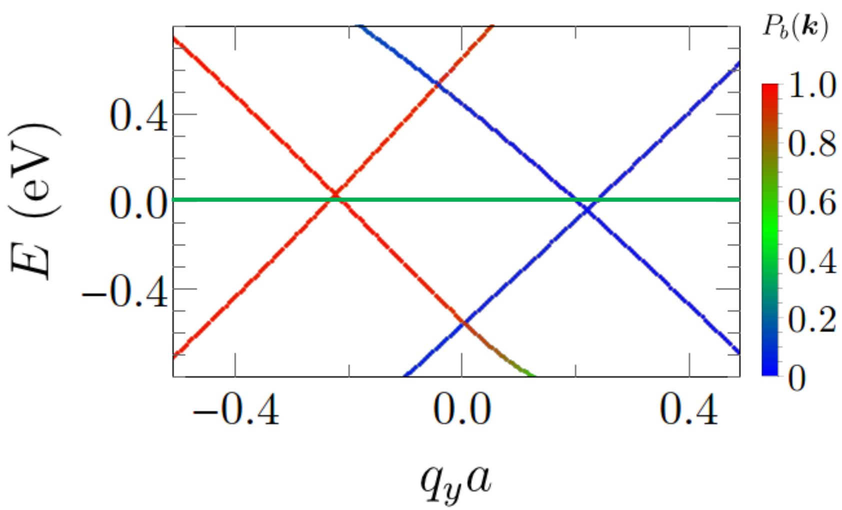
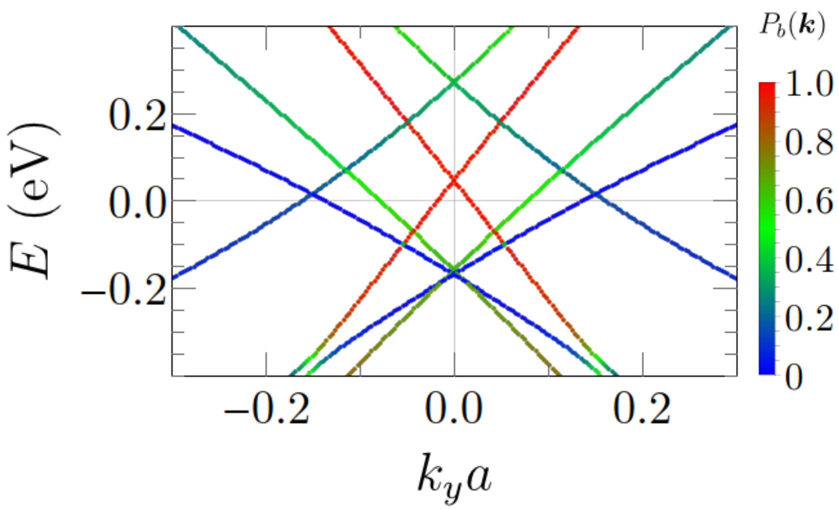


Zigzag

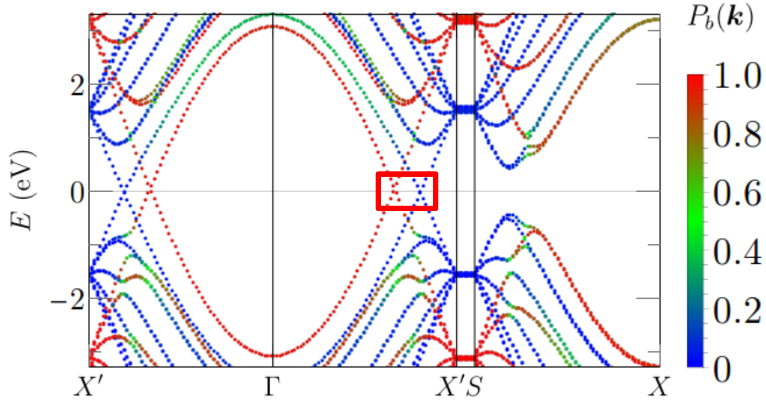




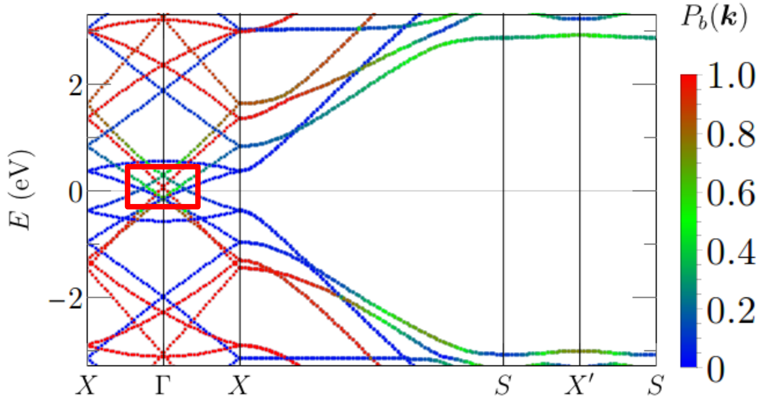


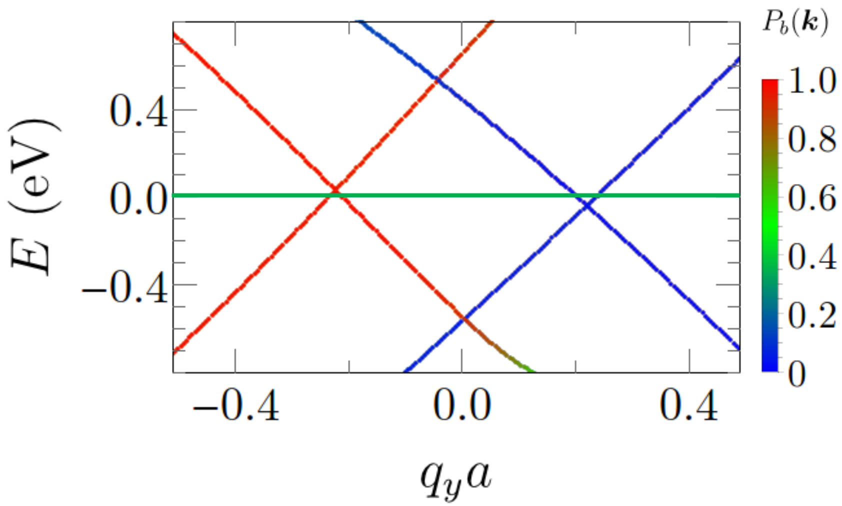
Uniaxial strain

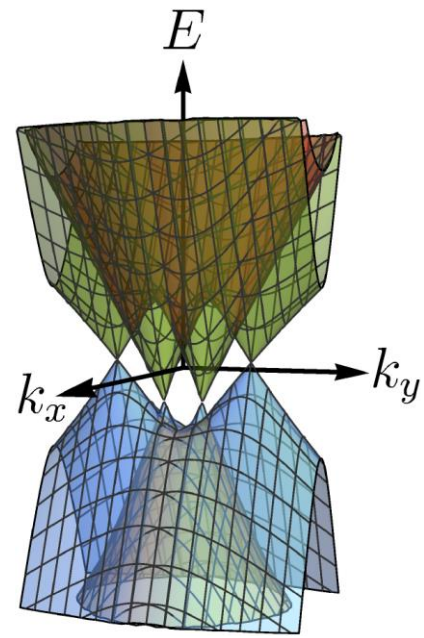
Armchair



Zigzag







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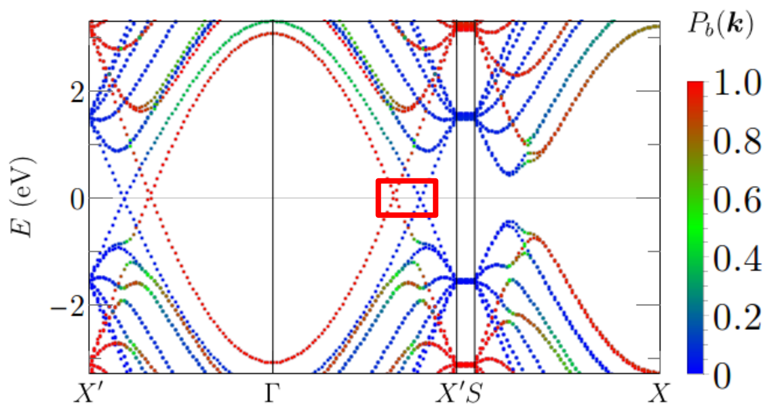

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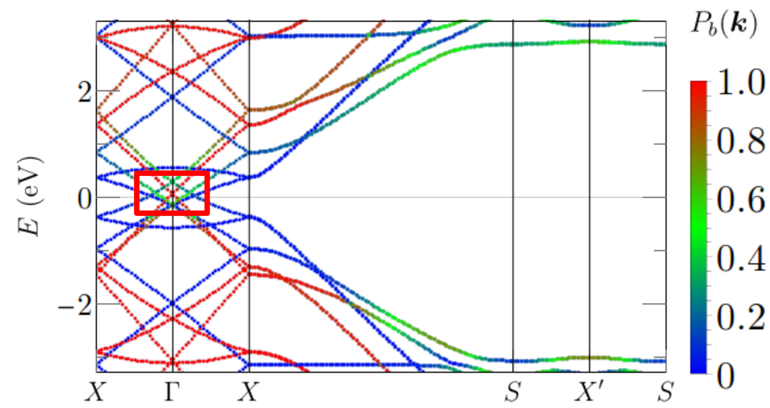

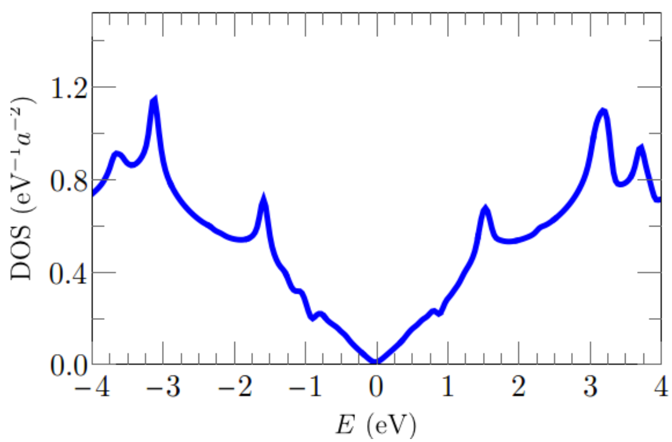

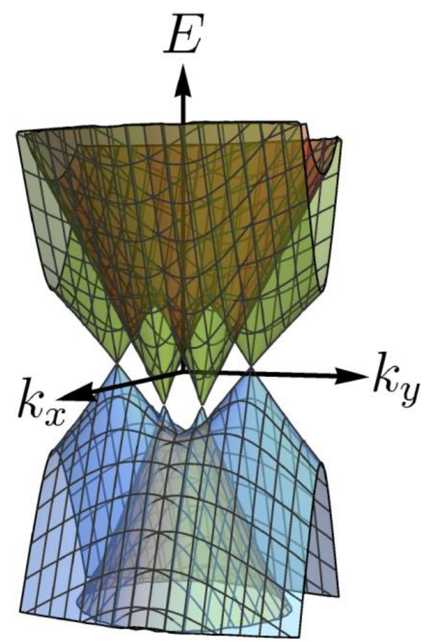

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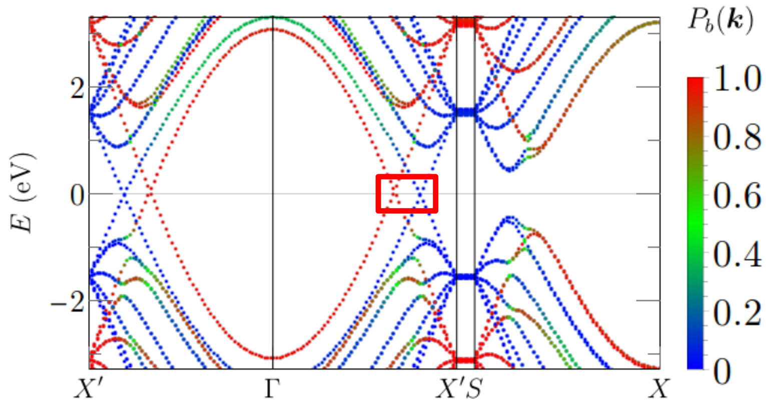
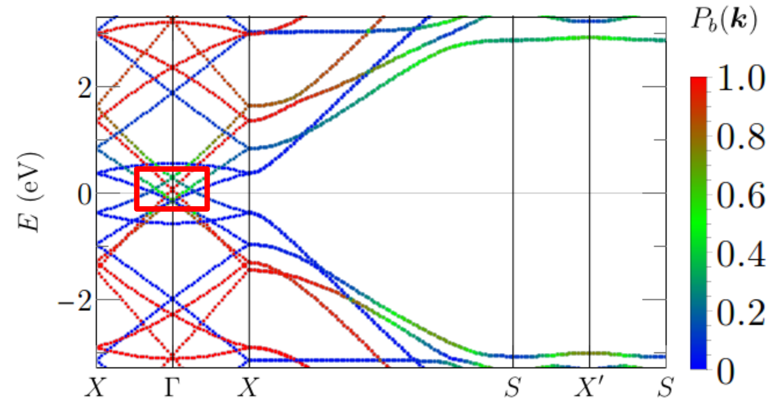
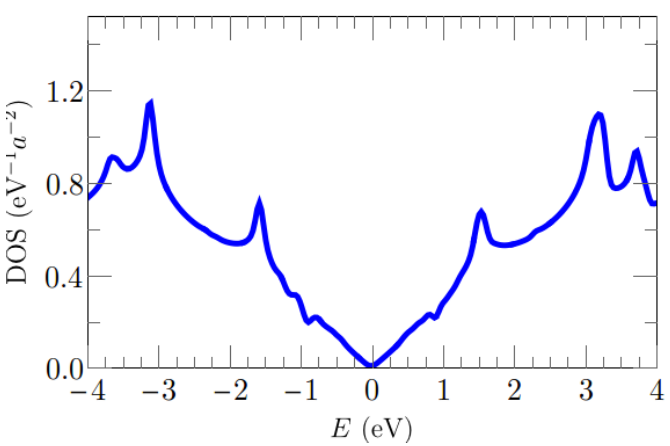
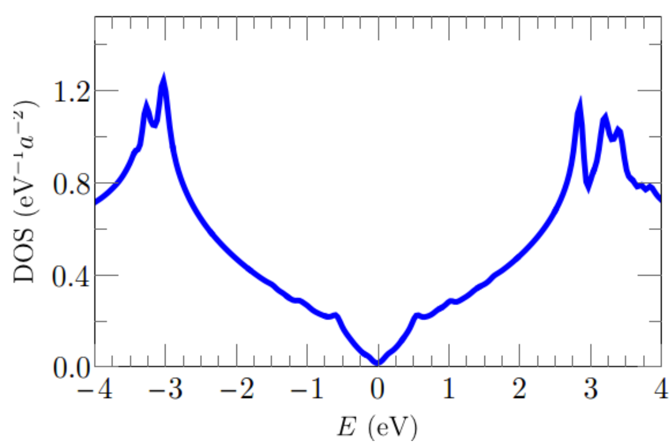


Zigzag







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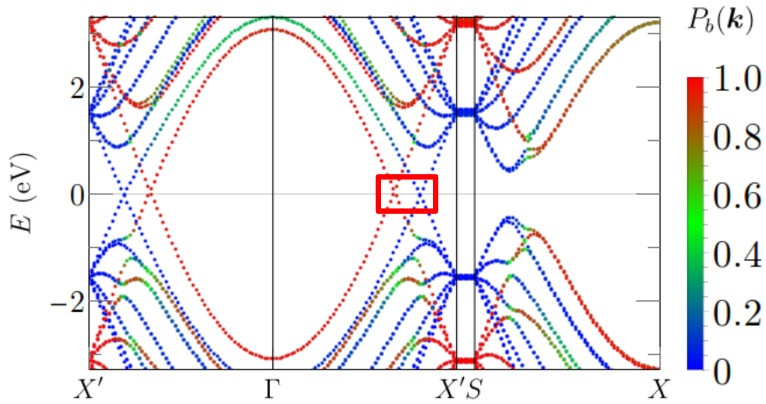

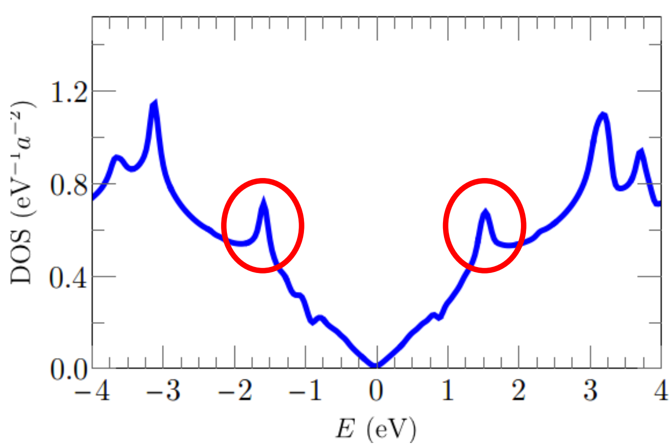

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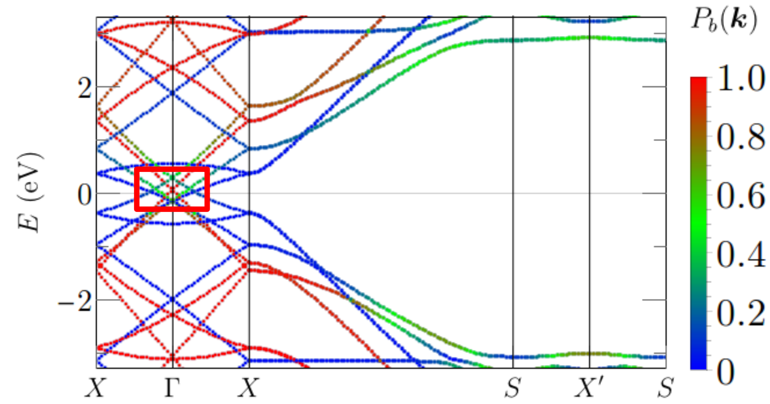

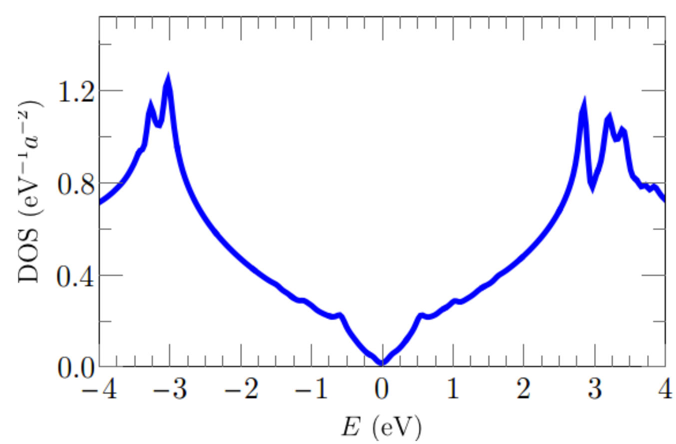

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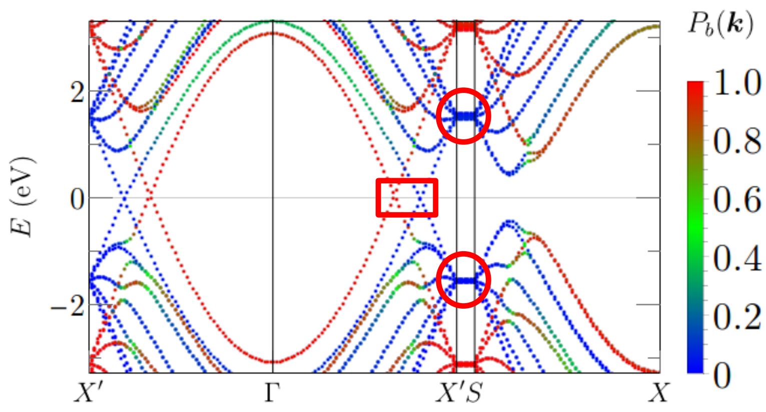

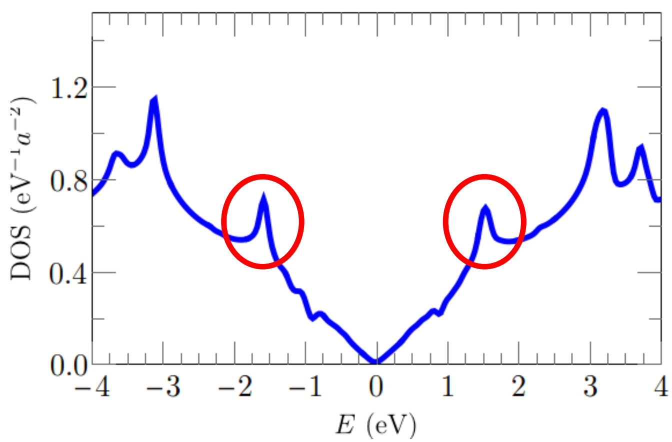

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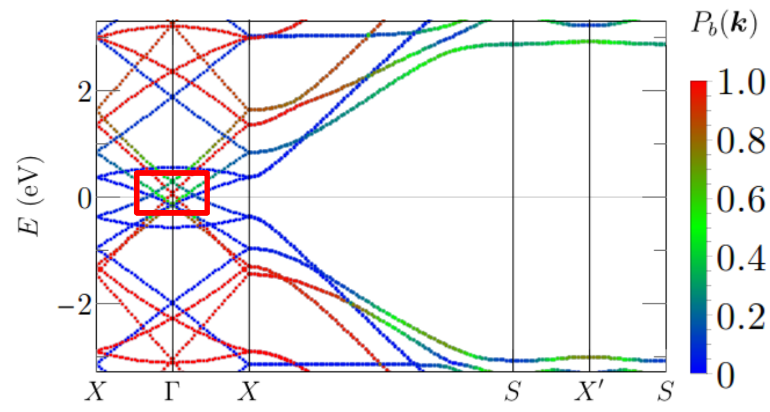

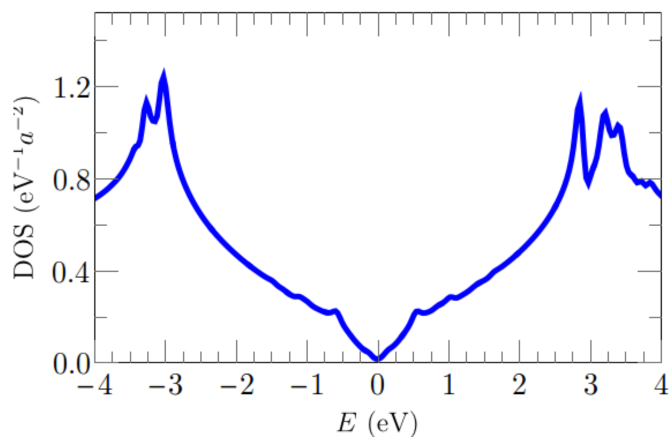

Summary and conclusions

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  ➡ General theory based on an expansion in Bloch states

- Known results for twisted bilayer graphene + dependence on rotation center, no piezoelectric effect

- Triaxial stress on one of the layers leads to charge transfer between the layers ➡ piezoelectric effect

- Uniaxial stress on one of the layers leads to a similar effect but depends on the direction of the stress