Pybinding homework 1, building the unit cell

Rectangular and honeycomb lattices

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Problem 1. Modify the square lattice given in pybinding notebook by adding a second B basis atom displaced at an arbitrary $\vec{b} = (b_x, b_y)$ of your choice. Define the $A \to B$ hopping term to be $t' = 2$. Represent graphically the resulting lattice.

Problem 2. Write a short function to generate a square lattice with an arbitrary basis atom B whose relative position with respect to A can be defined at input. Plot the resulting lattices for two arbitrary choices of $\vec{b}$.

Problem 3. What are the definitions of a reciprocal lattice and a Brillouin zone? Write down the formulas that relate the lattice vectors with the corresponding reciprocal lattice. Calculate the area of the Brillouin zone of the square lattice in Problem 1.

Problem 4. Modify the following example code provided in the python notebook

```
"""Create and plot a monolayer graphene lattice and it's Brillouin zone"""
import pybinding as pb
import matplotlib.pyplot as plt
from math import sqrt

pb.pltutils.use_style()


def monolayer_graphene():
    """Return the lattice specification for monolayer graphene"""
    a = 0.24595   # [nm] unit cell length
    a_cc = 0.142  # [nm] carbon-carbon distance
    t = -2.8      # [eV] nearest neighbour hopping

    # create a lattice with 2 primitive vectors
    lat = pb.Lattice(
        a1=[a, 0],
        a2=[a/2, a/2 * sqrt(3)]
    )

    lat.add_sublattices(
        # name and position
        ('A', [0, -a_cc/2]),
```

```
        ('B', [0,  a_cc/2])
    )

    lat.add_hoppings(
        # inside the main cell
        ([0,  0], 'A', 'B', t),
        # between neighboring cells
        ([1, -1], 'A', 'B', t),
        ([0, -1], 'A', 'B', t)
    )

    return lat


lattice = monolayer_graphene()
lattice.plot()
plt.show()
```

such that it generates automatically the lattice vector of a rectangular lattice with lattice vectors $\vec{a}_1 = (2, 0)$ and $\vec{a}_2 = (0, 1)$ with and without a basis atom B. Illustrate the resulting lattice and the associated Brillouin zone.