Graphene_nanoribbon

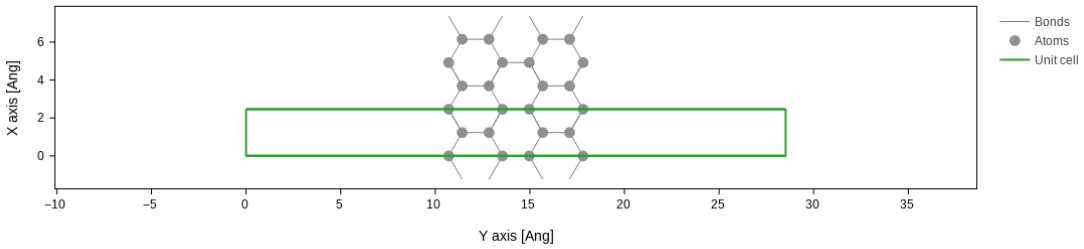
June 28, 2024

0.0.1 Graphene nanoribbon

[1]:
```
import sisl
import sisl.viz
import numpy as np
import plotly.express as px
```

Primer creem l'estructura del nanoribbon zigzag de grafè.

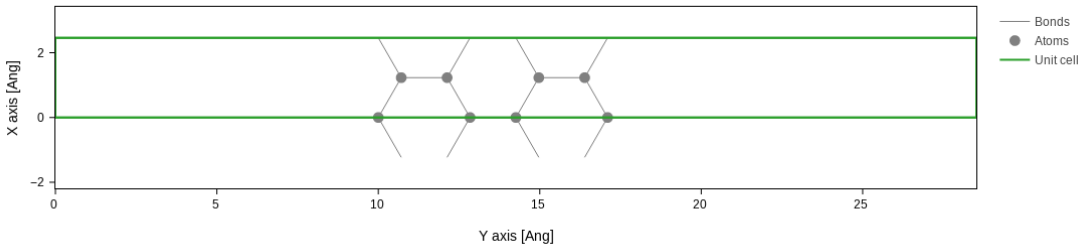
[2]:
```
nanoribbon_graphene1=sisl.geom.graphene_nanoribbon(width=4, bond=1.42,␣
↪kind='zigzag')
nanoribbon_graphene1.plot(nsc=[3,1,1], axes="yx")
```



[6]:
```
nanoribbon_graphene1
```

[6]:
```
<sisl.Geometry na=8, no=8, nsc=[3 1 1]>
```

[3]:
```
geometry1=sisl.Geometry.new(nanoribbon_graphene1)
geometry1.plot(axes="yx")
```



[133]:
```
geometry1.write('nanoribbon_graphene1.fdf')
```

[3]:
```
H1 = sisl.get_sile("inputs1/nanoribbon_graphene1.fdf").read_hamiltonian()
H1
```

[3]:
```
<sisl.physics.Hamiltonian na=8, no=104, nsc=[5 1 1], dim=2, nnz=36476,
spin=unpolarized>
```

[5]:
```
eigenstate1 = H1.eigenstate()
print('Els valors propis son:')
eigenstate1.eig
```

```
Els valors propis son:
```

[5]:
```
array([-1.85525066e+01, -1.76105318e+01, -1.60443065e+01, -1.41346689e+01,
       -1.08898119e+01, -7.88294156e+00, -6.63375014e+00, -5.58852864e+00,
       -5.56365542e+00, -4.70595748e+00, -4.65851807e+00, -4.01483613e+00,
       -3.58387054e+00, -2.73407581e+00, -2.40519321e+00, -1.54843780e-02,
        3.10098563e-01,  3.52343457e+00,  6.16520533e+00,  8.26457716e+00,
        8.70590752e+00,  9.09197419e+00,  9.89968484e+00,  9.99921803e+00,
        1.00135492e+01,  1.14104161e+01,  1.21148528e+01,  1.27964743e+01,
        1.30833173e+01,  1.41355585e+01,  1.46929925e+01,  1.61565430e+01,
        1.61760069e+01,  1.62296260e+01,  1.63193001e+01,  1.65386165e+01,
        1.70476698e+01,  1.73506254e+01,  1.76131624e+01,  1.76668295e+01,
        1.79801488e+01,  1.93348521e+01,  2.06279484e+01,  2.11150021e+01,
        2.27207745e+01,  2.49727438e+01,  2.57005398e+01,  2.64453658e+01,
        2.64883804e+01,  2.68779887e+01,  2.88508329e+01,  2.97606426e+01,
        3.14601765e+01,  3.22652814e+01,  3.27091976e+01,  3.28377057e+01,
        3.33662067e+01,  3.42031961e+01,  3.48940596e+01,  3.69083883e+01,
        3.70315506e+01,  3.84305629e+01,  4.01981081e+01,  4.18002168e+01,
        4.41084777e+01,  4.56010852e+01,  4.76463110e+01,  4.89930642e+01,
        4.97097821e+01,  5.01765215e+01,  5.04490826e+01,  5.05382196e+01,
        5.23275211e+01,  5.33586348e+01,  5.36392608e+01,  5.59725183e+01,
        5.64863824e+01,  5.65088273e+01,  5.71369957e+01,  5.94191500e+01,
```

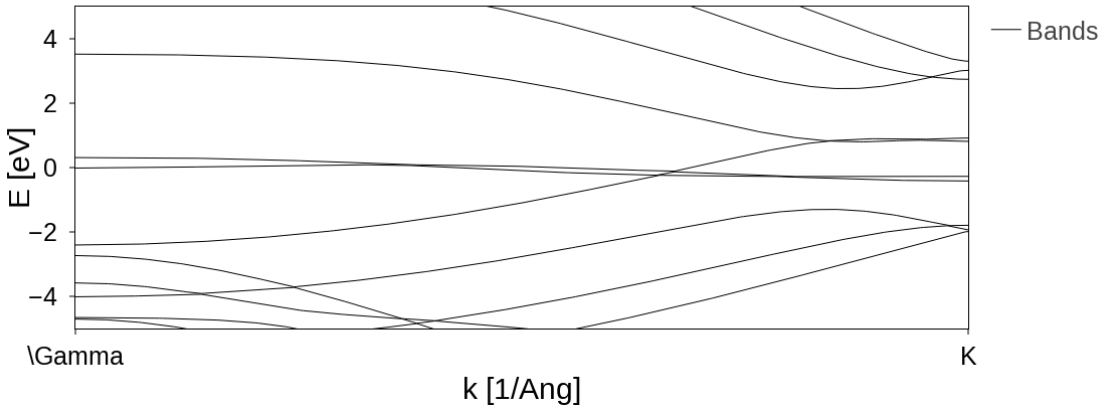
```
       5.97057784e+01,  6.12760742e+01,  6.29664782e+01,  6.63396956e+01,
       6.85255013e+01,  7.15881740e+01,  7.17766516e+01,  7.19563304e+01,
       7.39934075e+01,  7.43067029e+01,  7.59552548e+01,  7.85019915e+01,
       7.90133889e+01,  8.01334047e+01,  8.14654538e+01,  8.40585875e+01,
       8.87801330e+01,  9.38780912e+01,  1.02588563e+02,  1.05202534e+02,
       1.07306071e+02,  1.22539154e+02,  1.40868863e+02,  1.41165506e+02])
```

[6]:
```
eigenstate1 = H1.eigenstate()
print('La matriu dels coeficients dels estats propis son:')
eigenstate1.state
```

```
La matriu dels coeficients dels estats propis son:
```

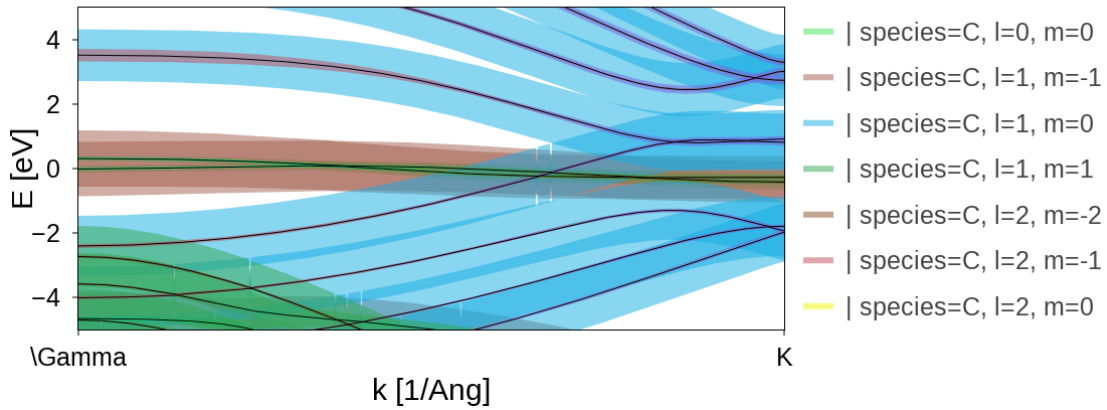
[6]:
```
array([[-1.33771221e-01,  2.56940066e-03,  1.53507625e-02, …,
         2.47619256e-03,  3.07147208e-18,  2.64837732e-03],
       [ 1.59539132e-01,  5.34441482e-02, -1.27467976e-03, …,
         8.49527036e-04,  2.30004828e-17, -2.76140911e-03],
       [-1.74260320e-01, -9.31680338e-02, -3.22121397e-02, …,
        -1.38494681e-04,  5.05097562e-17, -1.29927956e-02],
       …,
       [-3.68115784e-08,  2.72523682e-08, -5.74601614e-09, …,
         2.60108294e-08,  1.96519578e-11,  4.32870115e-08],
       [-9.20208020e-02,  2.00754022e-01,  5.34039763e-01, …,
        -8.05723780e-01,  2.37685831e-15, -4.89449276e-01],
       [ 1.22338162e-07, -2.30022793e-07, -5.78594422e-07, …,
         8.79519974e-07, -1.15104601e-11,  5.20032769e-07]])
```

[10]:
```
band_struct1=sisl.BandStructure(H1, points=[[0,0,0],[0,0,0],[0.5,0,0]],␣
 ↪divisions=300, names=[r"\Gamma", "M", "K"])
band_struct1.plot().update_layout(height=500, yaxis=dict(range=[-5, 5]),␣
 ↪font_size=25)
```

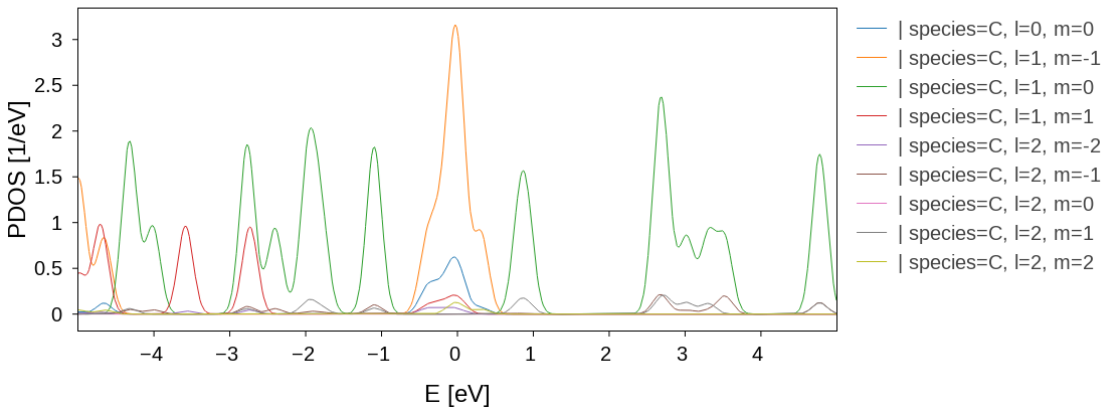


Representem les Fatbands i PDOS i mirem les contribucions dels orbitals:

[11]:
```
fatbands1 = band_struct1.plot.fatbands()
fatbands1.split_groups(on="species+l+m", scale=2)
fatbands1.update_layout(height=500, yaxis=dict(range=[-5, 5]), font_size=25)
```

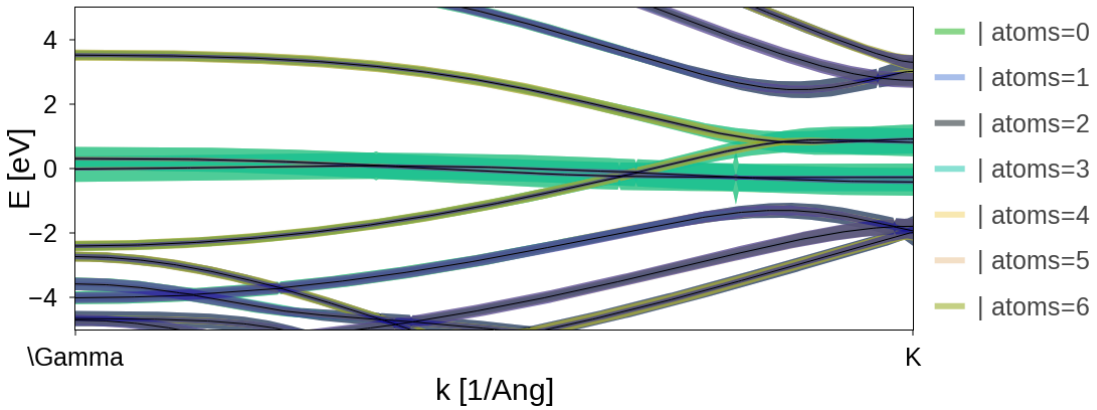


[15]:
```
pdos_plot1 = H1.plot.pdos(
    kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10], Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1)
)

pdos_plot1.split_DOS(on="species+l+m")
pdos_plot1.update_layout(height=500, font_size=20)
```

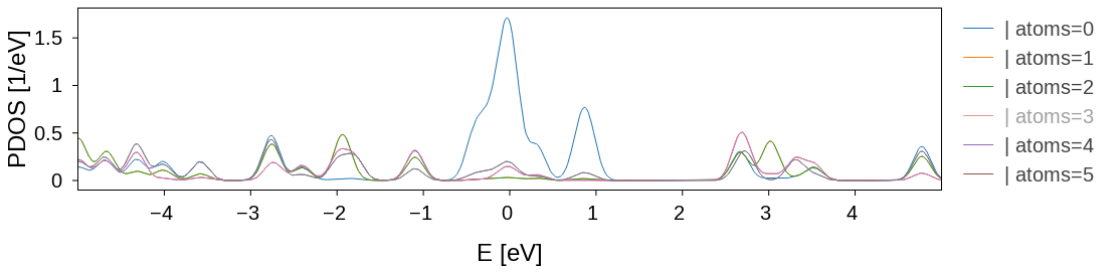


Representem les Fatbands i PDOS i mirem les contribucions dels àtoms:

[16]:
```
fatbands1A = band_struct1.plot.fatbands()
fatbands1A.split_groups(on="atoms", scale=2)
fatbands1A.update_layout(height=500, yaxis=dict(range=[-5, 5]), font_size=25)
```

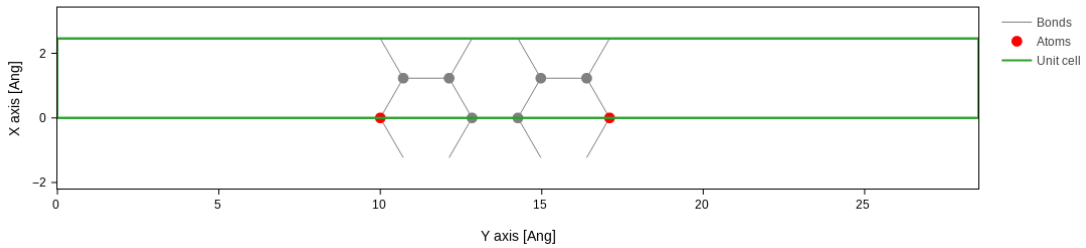


[17]:
```
pdos_plot1A = H1.plot.pdos(
    kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10], Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1)
)

pdos_plot1A.split_DOS(on="atoms")
pdos_plot1A.update_layout(height=500, font_size=20)
```



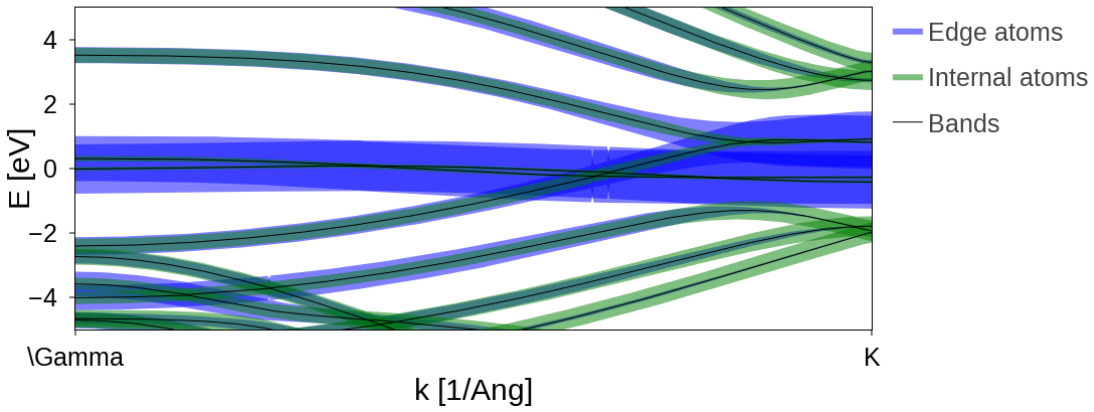
Veiem que els àtoms 0 i 3 son els que més contribueixen als estats que no haurien d'apareixer a prop del nivell de fermi.

[15]:
```
nanoribbon_graphene1.plot(axes="yx", atoms_style=[{"atoms": [0,3], "color":"red"}])
```



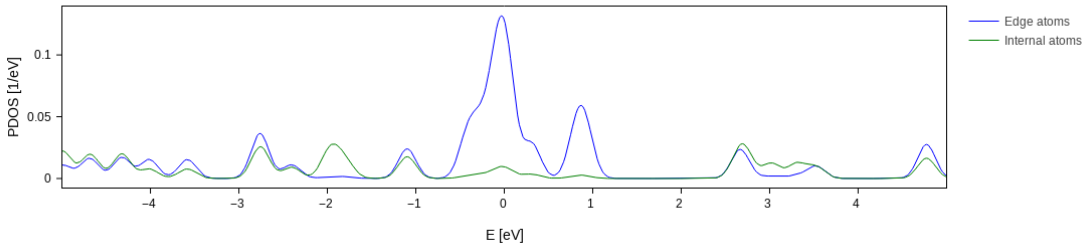
Podem veure millor les contribucions dels àtoms externs i interns.

[18]:
```
fatbands1 = band_struct1.plot.fatbands(groups = [{"name":"Edge atoms", "atoms":[0,3], "color": "blue", "reduce": "mean"},
                                                 {"name": "Internal atoms","atoms": [1,2,4,5,6,7], "color": "green", "reduce": "mean"}],
                                       fatbands_scale=50)

fatbands1.update_layout(height=500, yaxis=dict(range=[-5, 5]), font_size=25)
```

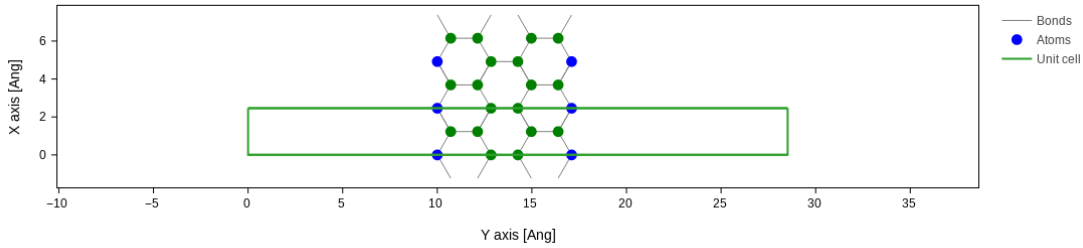


[51]:
```
PDOS_H1 = H1.plot.pdos(
    kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10], Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1),
```

```
    groups = [{"name":"Edge atoms", "atoms": [0,3], "color": "blue", "reduce":␣
 ↪"mean"},
                                                {"name": "Internal atoms",␣
 ↪"atoms": [1,2,4,5,6,7], "color": "green", "reduce": "mean"}]
)
PDOS_H1
```

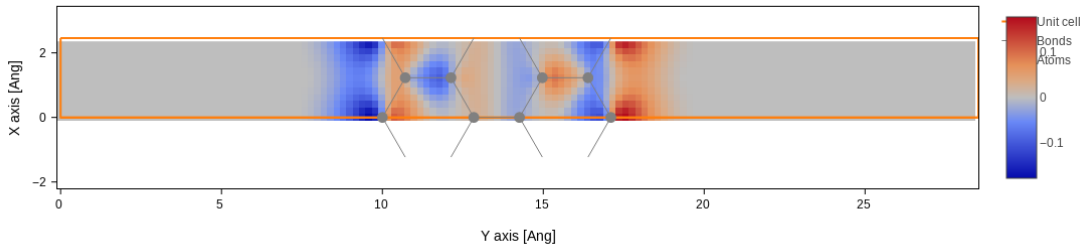


[55]:
```
nanoribbon_graphene1.plot(nsc=[3,1,1], axes="yx", atoms_style=[{"atoms": [0,3],␣
 ↪"color": "blue"}, {"atoms": [1,2,4,5,6,7], "color": "green"}])
```

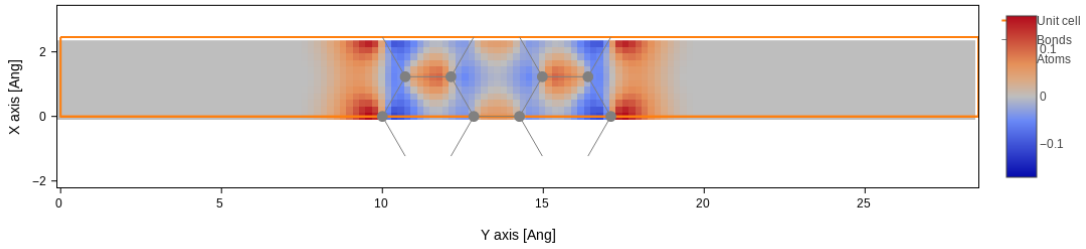


Plotegem les funcions d'ona d'aquestes bandes.

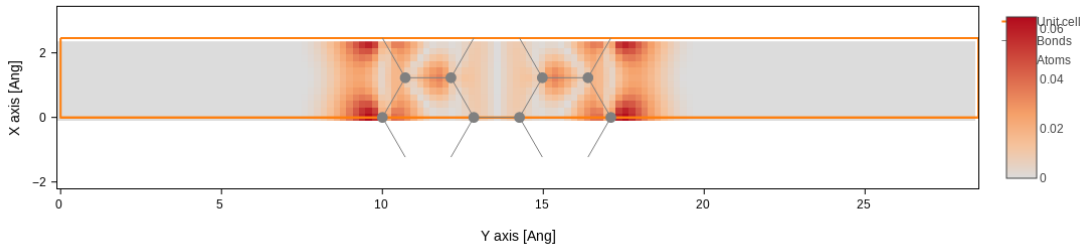
[104]:
```
H1.plot.wavefunction(i=15, axes="yx", z_range=[0,3], plot_geom=True, cmid=0)
```



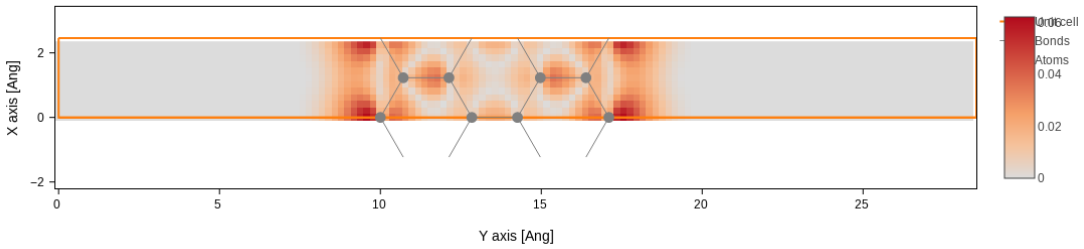
[102]:
```
H1.plot.wavefunction(i=16, axes="yx", z_range=[0,3], plot_geom=True, cmid=0)
```



[96]:
```
H1.plot.wavefunction(i=15, axes="yx", represent="mod", plot_geom=True)
```



[100]:
```
H1.plot.wavefunction(i=16, axes="yx", represent="mod", plot_geom=True)
```



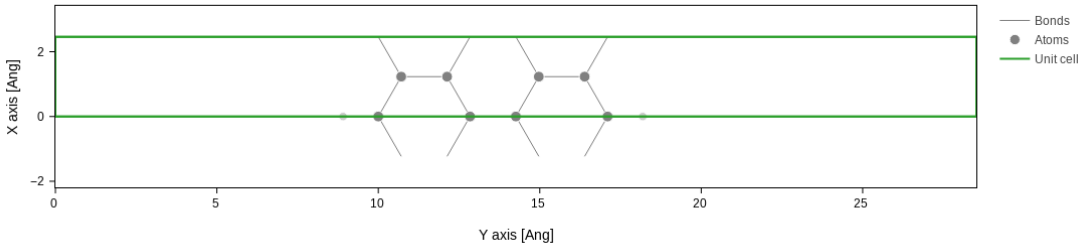
Veiem que l'aparició dels estats no desitjats a l'estrucutura de bandes és degut als carbonis dels extrems del nanoribbon, aquests carbonis tenen un electró lliure i per tant surten unes bandes gairebé planes. Per fer desapareixer aquestes bandes, afegim hidrogens per formar un parell d'electrons. La distància d'enllacç entre C i H és 1,09 Ang. Afegim dos àtoms d'H enllaçats als C 1 i 4 en el fitxer .fdf.

[20]:
```
H2 = sisl.get_sile("inputs2/nanoribbon_graphene2.fdf").read_hamiltonian()
H2
```

[20]:
```
<sisl.physics.Hamiltonian na=10, no=114, nsc=[5 1 1], dim=2, nnz=41894,
spin=unpolarized>
```

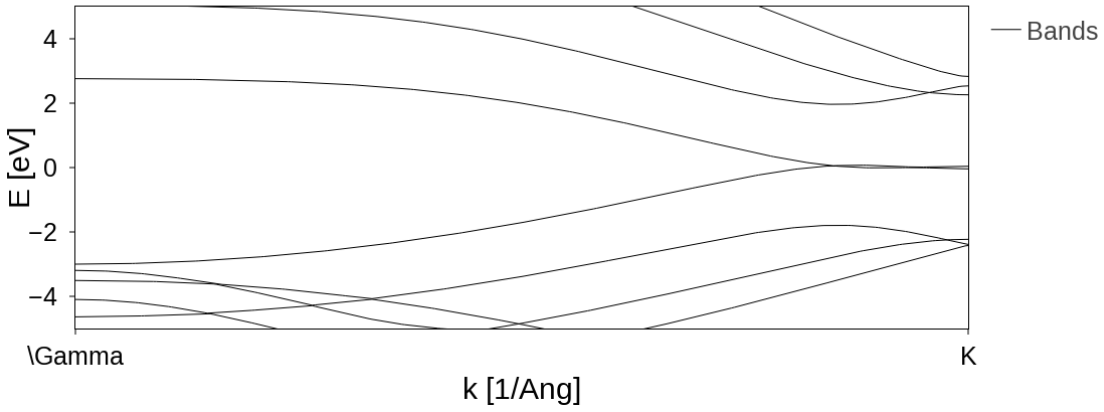
Mirem l'estructura del nanoribbon per veure si hem afegit bé els hidrogens.

[26]:
```
geomH2 = sisl.get_sile("inputs2/nanoribbon_graphene2.fdf").read_geometry()
geomH2.plot(axes="yx")
```

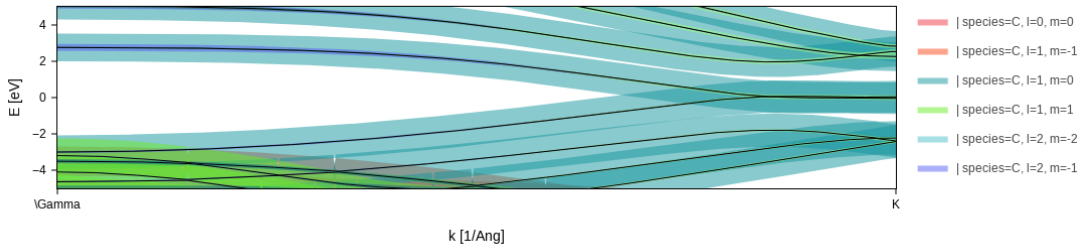


[21]:
```
band_struct2=sisl.BandStructure(H2, points=[[0,0,0],[0,0,0],[0.5,0,0]],␣
↪divisions=300, names=[r"\Gamma", "M", "K"])
bands_plot2=band_struct2.plot().update_layout(height=500, yaxis=dict(range=[-5,␣
↪5]), font_size=25)
```

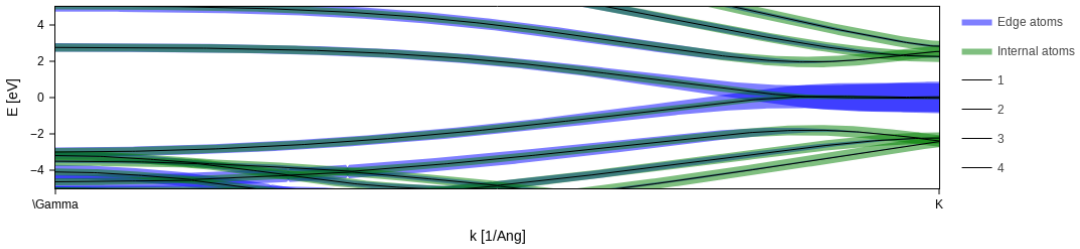
```
bands_plot2
```



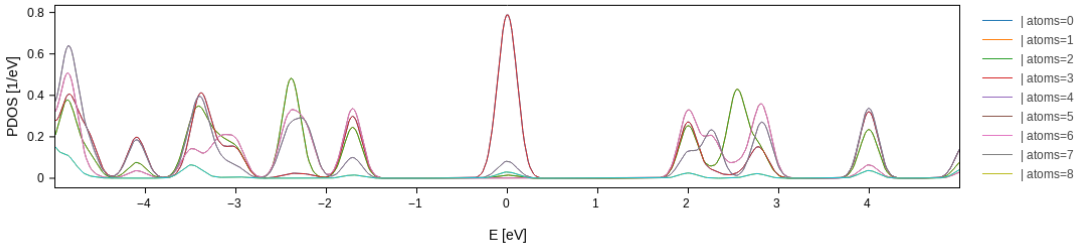
[112]:
```
fatbands2 = band_struct2.plot.fatbands()
fatbands2.split_groups(on="species+l+m", scale=2)
fatbands2.update_layout(height=500, yaxis=dict(range=[-5, 5]))
```



[107]:
```
fatbands2 = band_struct2.plot.fatbands(groups = [{"name":"Edge atoms", "atoms":␣
↪[0,3], "color": "blue", "reduce": "mean"},
                                                 {"name": "Internal atoms",␣
↪"atoms": [1,2,4,5,6,7], "color": "green", "reduce": "mean"}],
                                        fatbands_scale=50)
fatbands2.update_layout(height=500, yaxis=dict(range=[-5, 5]))
```



[105]:
```
PDOS_H2 = H2.plot.pdos(kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10],␣
↪Erange=[-5,5],
   distribution=sisl.get_distribution(method="gaussian", smearing=0.1))

PDOS_H2.split_DOS(on="atoms")
```

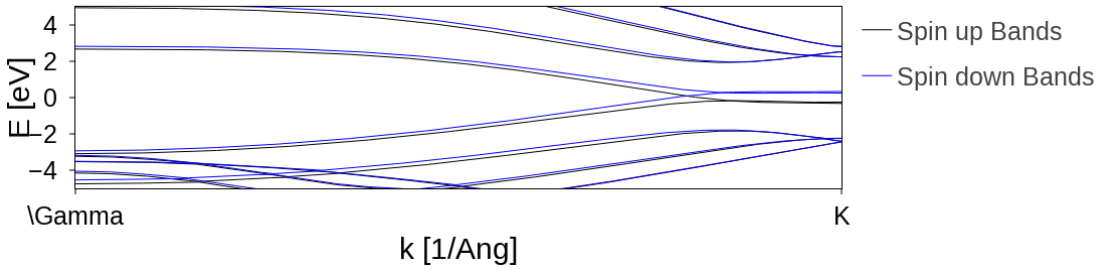


Ara afegim una polarització de l'spin.

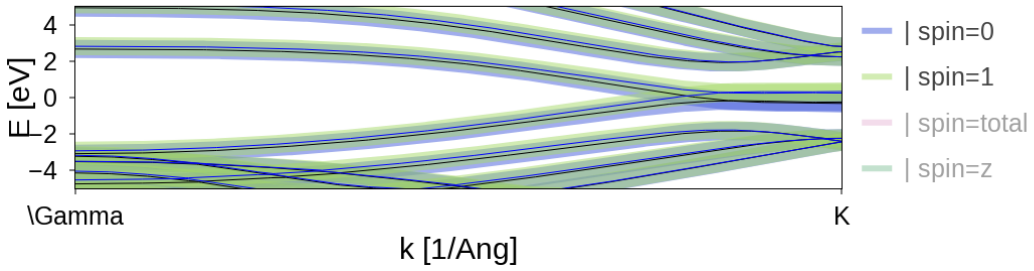
[22]:
```
H3 = sisl.get_sile("inputs3/nanoribbon_graphene3.fdf").read_hamiltonian()
H3
```

[22]:
```
<sisl.physics.Hamiltonian na=10, no=114, nsc=[5 1 1], dim=3, nnz=41894,
spin=polarized>
```

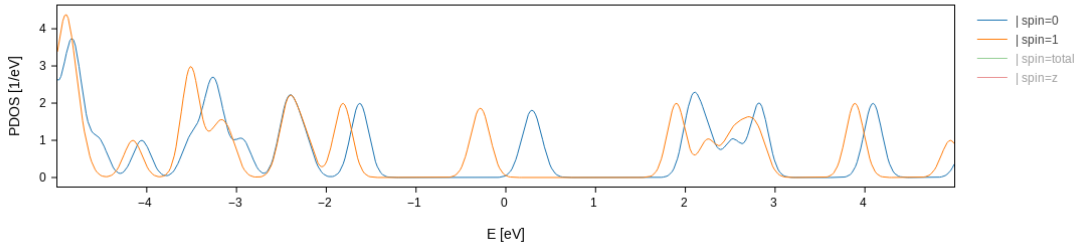
[23]:
```
band_struct3=sisl.BandStructure(H3, points=[[0,0,0],[0,0,0],[0.5,0,0]],␣
↪divisions=300, names=[r"\Gamma", "M", "K"])
bands_plot3=band_struct3.plot().update_layout(height=500, yaxis=dict(range=[-5,␣
↪5]), font_size=25)
bands_plot3
```



[38]:
```
fatbands3=band_struct3.plot.fatbands()
fatbands3.split_groups(on="spin")
fatbands3.update_layout(height=500, yaxis=dict(range=[-5, 5]), font_size=25)
```



[32]:
```
PDOS_H3 = H3.plot.pdos(
    kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10], Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1)
)
PDOS_H3.split_DOS(on="spin")
```

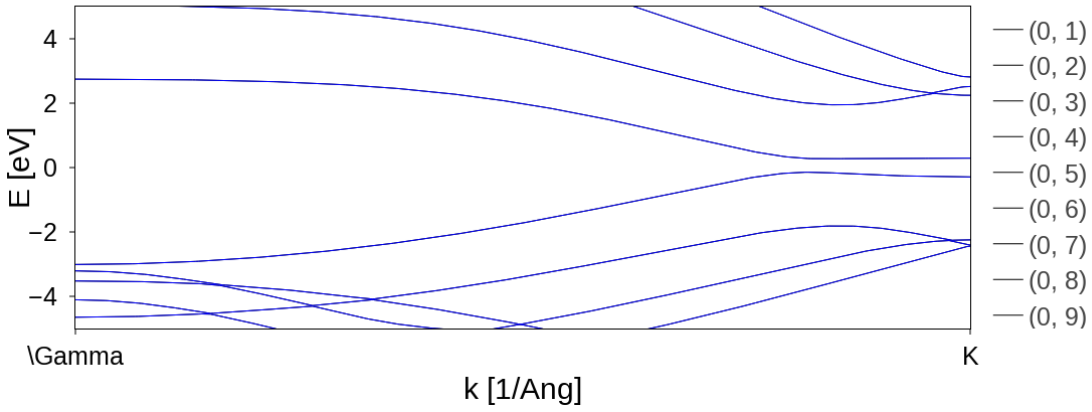


Forcem una configuració AF.

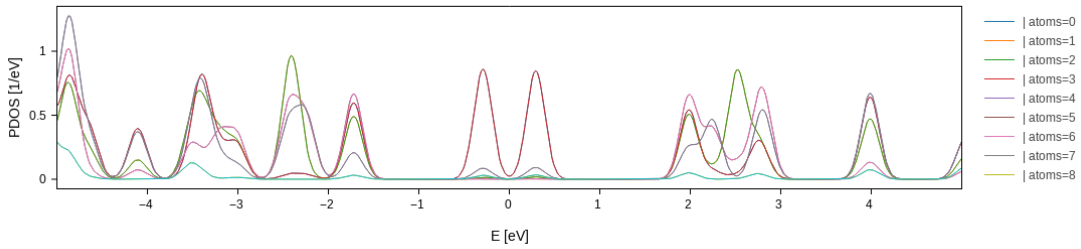
[2]:
```
H4 = sisl.get_sile("inputs4/nanoribbon_graphene4.fdf").read_hamiltonian()
H4
```

[2]:
```
<sisl.physics.Hamiltonian na=10, no=114, nsc=[5 1 1], dim=3, nnz=41894,
spin=polarized>
```

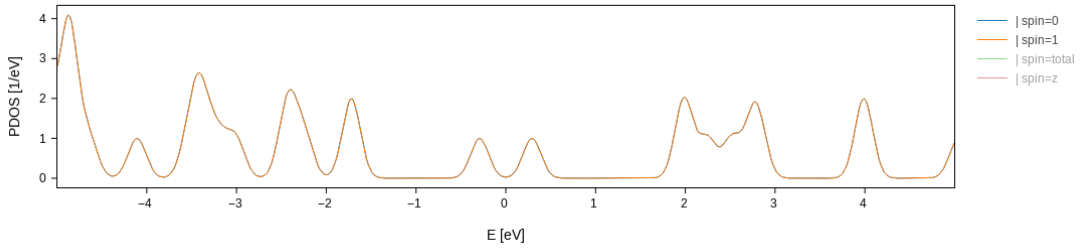
[3]:
```
band_struct4=sisl.BandStructure(H4, points=[[0,0,0],[0,0,0],[0.5,0,0]],␣
↪divisions=300, names=[r"\Gamma", "M", "K"])
bands_plot4=band_struct4.plot().update_layout(height=500, yaxis=dict(range=[-5,␣
↪5]), font_size=25)
bands_plot4
```



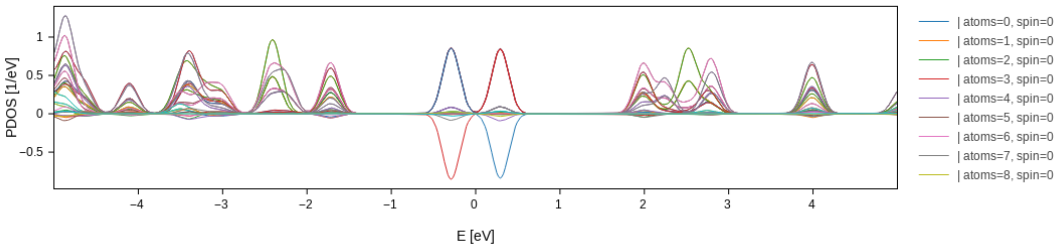
[5]:
```
PDOS_H4 = H4.plot.pdos(kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10],␣
↪Erange=[-5,5],
   distribution=sisl.get_distribution(method="gaussian", smearing=0.1))

PDOS_H4.split_DOS(on="atoms")
```



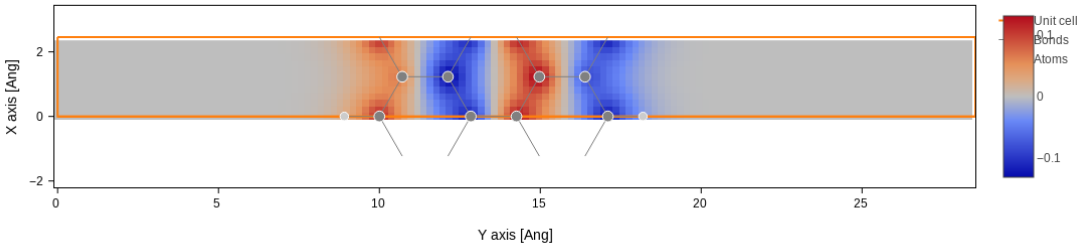
[16]:
```
PDOS_H4 = H4.plot.pdos(kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10],␣
↪Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1))

PDOS_H4.split_DOS(on="spin")
```



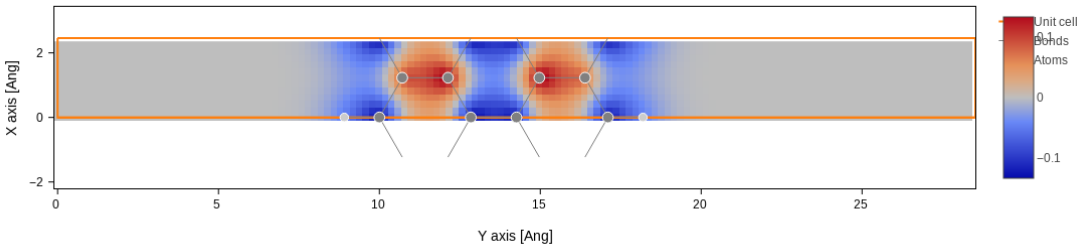
[9]:
```
PDOS_H4 = H4.plot.pdos(kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10],␣
↪Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1))

PDOS_H4.split_DOS(on="atoms+spin")
```



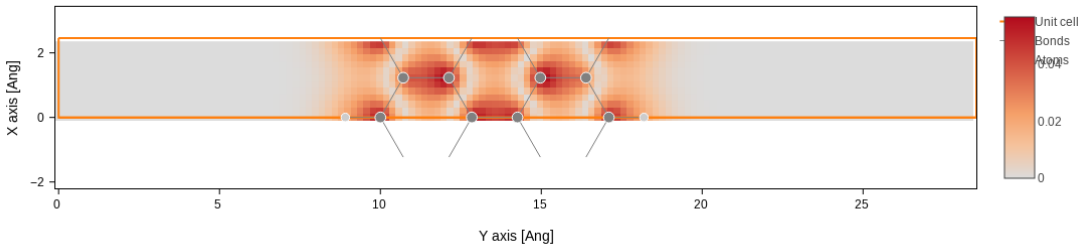
[18]:
```
H4.plot.wavefunction(i=16, axes="yx", z_range=[0,3], plot_geom=True, cmid=0)
```



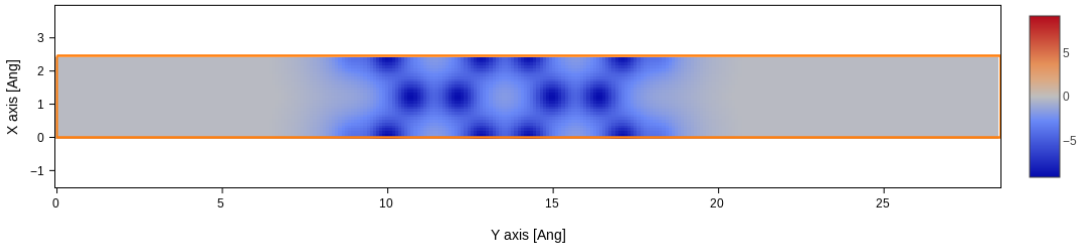
[25]:
```
H4.plot.wavefunction(i=17, axes="yx", z_range=[0,3], plot_geom=True, cmid=0)
```



[21]:
```
H4.plot.wavefunction(i=17, axes="yx", represent="mod", plot_geom=True)
```



[53]:
```
E4 = sisl.get_sile("inputs4/siesta.VT").plot(axes="yx", cmid=0)
E4
```

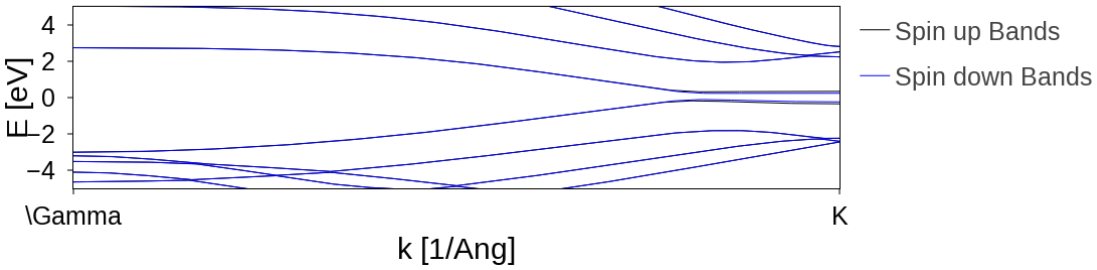


Ara provem d'aplicar un camp electric extern de 0.05 V/A.

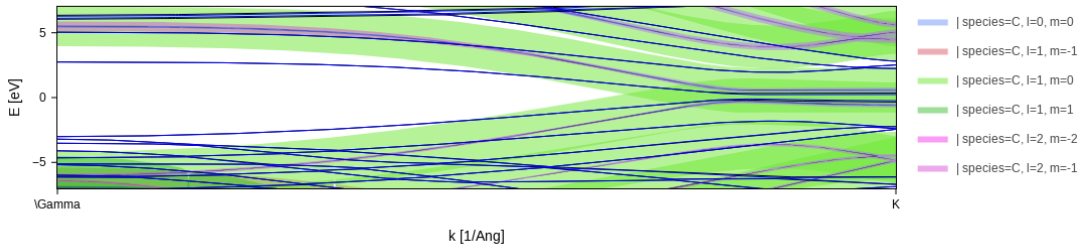
[10]:
```
H5 = sisl.get_sile("inputs5/nanoribbon_graphene5.fdf").read_hamiltonian()
H5
```

[10]:
```
<sisl.physics.Hamiltonian na=10, no=114, nsc=[5 1 1], dim=3, nnz=41894,
spin=polarized>
```

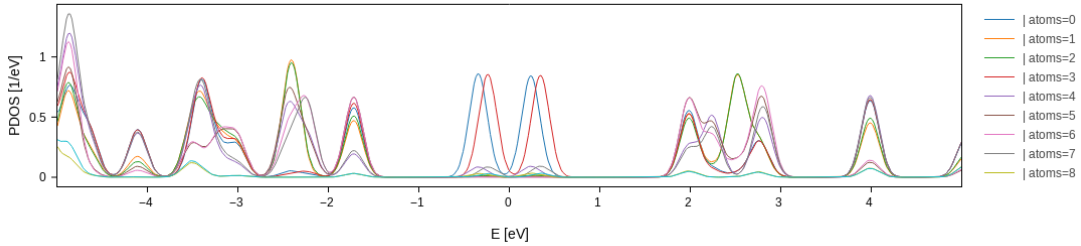
[43]:
```
band_struct5=sisl.BandStructure(H5, points=[[0,0,0],[0,0,0],[0.5,0,0]],␣
↪divisions=300, names=[r"\Gamma", "M", "K"])
bands_plot5=band_struct5.plot().update_layout(height=500, yaxis=dict(range=[-5,␣
↪5]), font_size=25)
bands_plot5
```



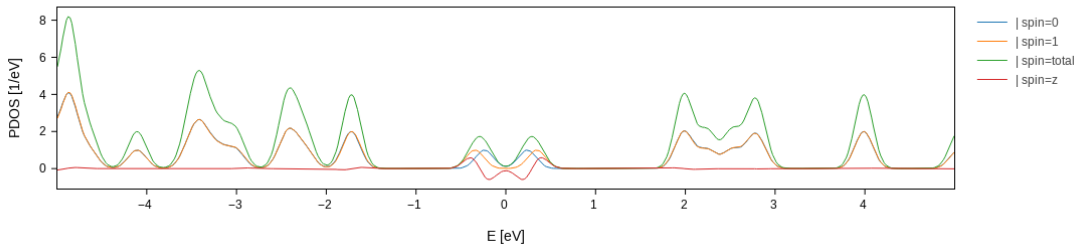
[50]:
```
fatbands5 = band_struct5.plot.fatbands()
fatbands5.split_groups(on="species+l+m", scale=2)
fatbands5.update_layout(height=500, yaxis=dict(range=[-7, 7]))
```



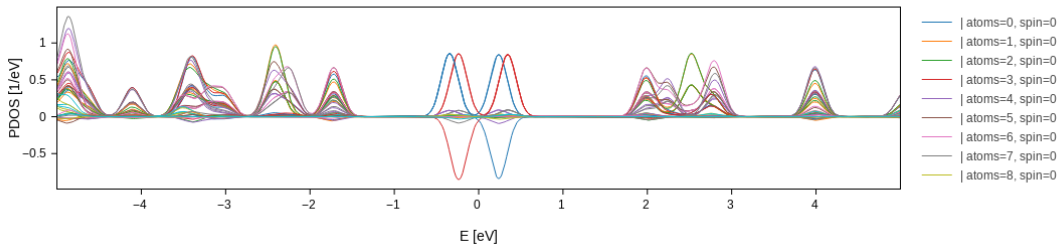
[51]:
```
PDOS_H5 = H5.plot.pdos(kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10],␣
↪Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1))

PDOS_H5.split_DOS(on="atoms")
```



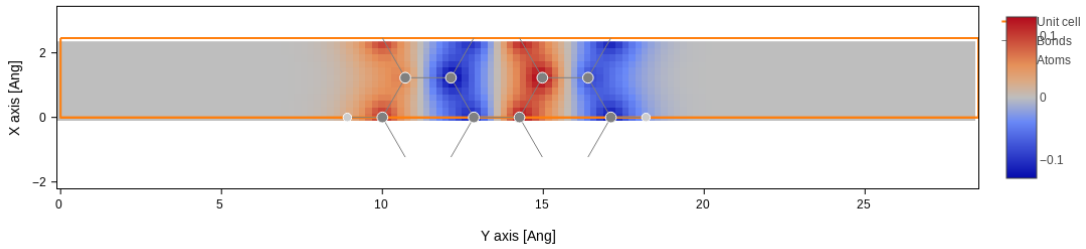
[15]:
```
PDOS_H5 = H5.plot.pdos(kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10],␣
↪Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1))

PDOS_H5.split_DOS(on="spin")
```



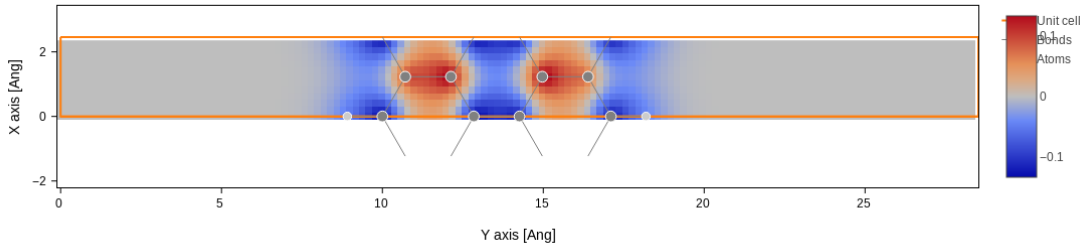
[11]:
```
PDOS_H5 = H5.plot.pdos(kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10],␣
↪Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1))

PDOS_H5.split_DOS(on="atoms+spin")
```



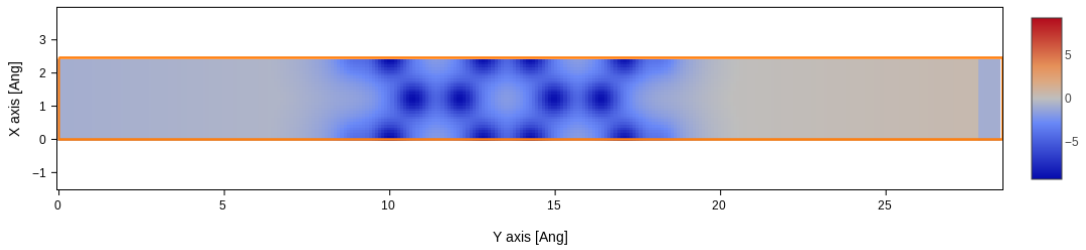
[52]:
```
H5.plot.wavefunction(i=16, axes="yx", z_range=[0,3], plot_geom=True, cmid=0)
```



[53]:
```
H5.plot.wavefunction(i=17, axes="yx", z_range=[0,3], plot_geom=True, cmid=0)
```



[49]:
```
E5 = sisl.get_sile("inputs5/siesta.VT").plot(axes="yx", cmid=0)
E5
```

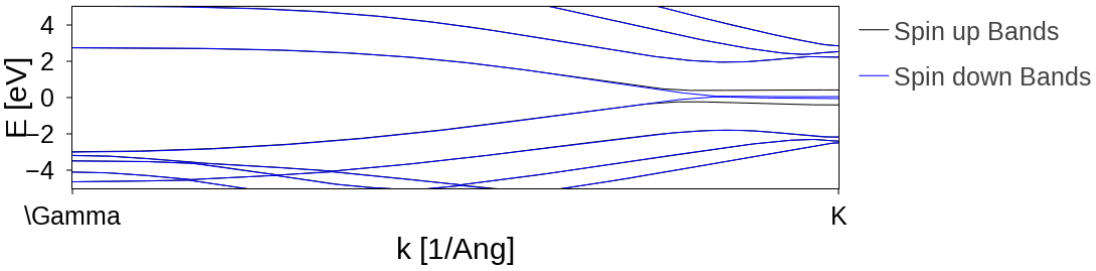


Provem un camp de 0.5 V/A.

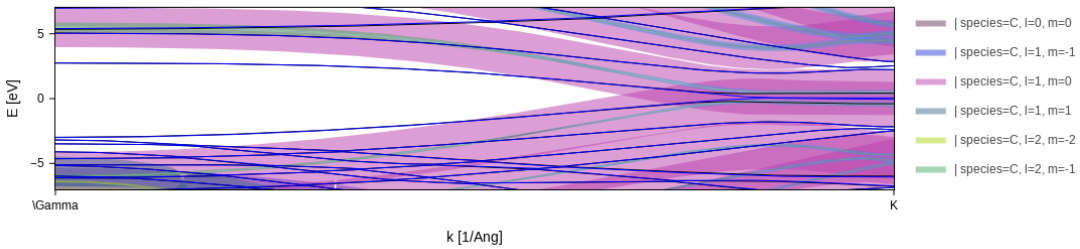
[12]:
```
H6 = sisl.get_sile("inputs6/nanoribbon_graphene6.fdf").read_hamiltonian()
H6
```

[12]:
```
<sisl.physics.Hamiltonian na=10, no=114, nsc=[5 1 1], dim=3, nnz=41894,
spin=polarized>
```

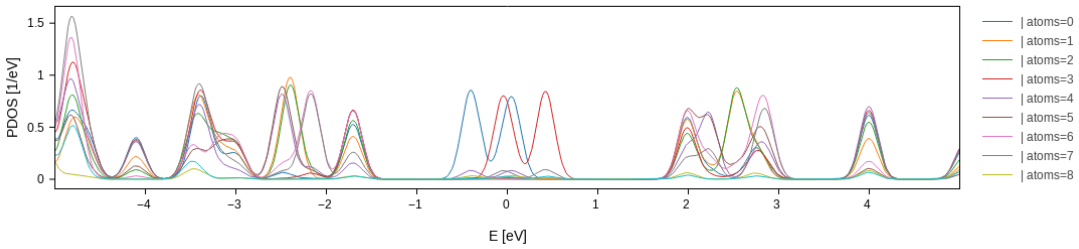
[46]:
```
band_struct6=sisl.BandStructure(H6, points=[[0,0,0],[0,0,0],[0.5,0,0]],␣
↪divisions=300, names=[r"\Gamma", "M", "K"])
bands_plot6=band_struct6.plot().update_layout(height=500, yaxis=dict(range=[-5,␣
↪5]), font_size=25)
bands_plot6
```



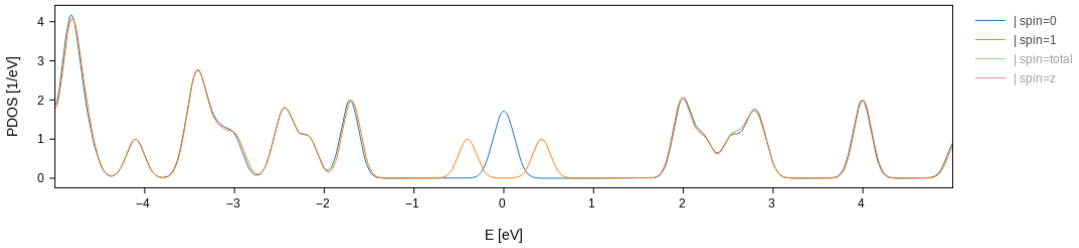
[59]:
```
fatbands6 = band_struct6.plot.fatbands()
fatbands6.split_groups(on="species+l+m", scale=2)
fatbands6.update_layout(height=500, yaxis=dict(range=[-7, 7]))
```



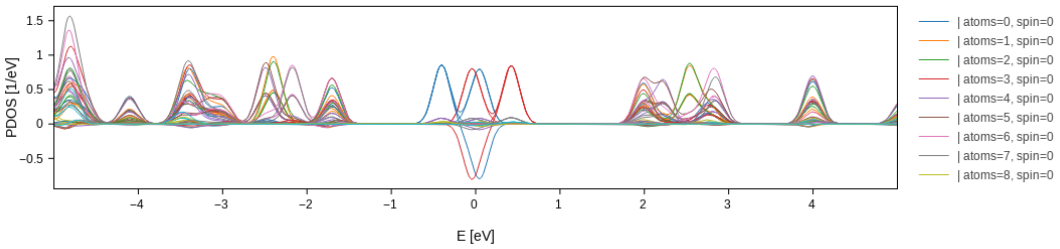
[60]:
```
PDOS_H6 = H6.plot.pdos(kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10],␣
↪Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1))

PDOS_H6.split_DOS(on="atoms")
```



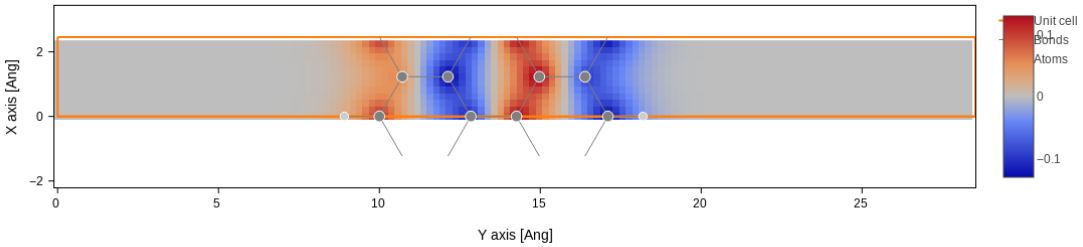
[14]:
```
PDOS_H6 = H6.plot.pdos(kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10],␣
↪Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1))

PDOS_H6.split_DOS(on="spin")
```



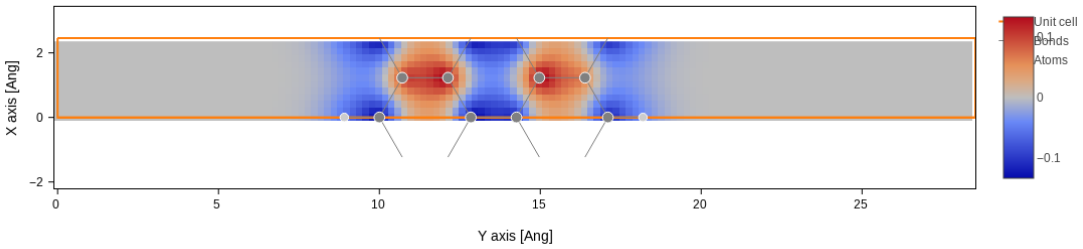
[13]:
```
PDOS_H6 = H6.plot.pdos(kgrid=[4,1,1], nE=1000, data_Erange=[-10, 10],␣
↪Erange=[-5,5],
    distribution=sisl.get_distribution(method="gaussian", smearing=0.1))

PDOS_H6.split_DOS(on="atoms+spin")
```



[61]:
```
H6.plot.wavefunction(i=16, axes="yx", z_range=[0,3], plot_geom=True, cmid=0)
```

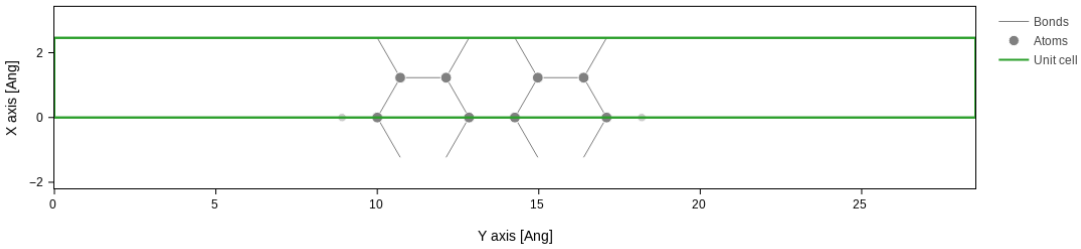


[62]:
```
H6.plot.wavefunction(i=17, axes="yx", z_range=[0,3], plot_geom=True, cmid=0)
```

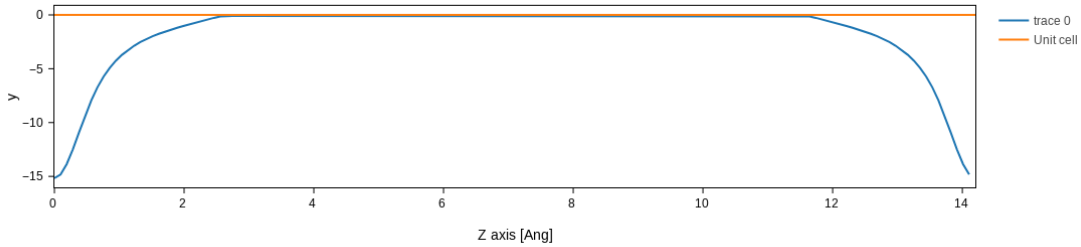


Mirem l'energia potencial.

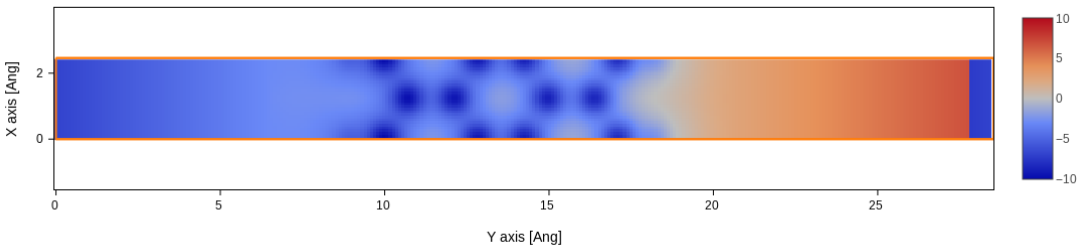
[27]:
```
geomH2.plot(axes="yx")
```



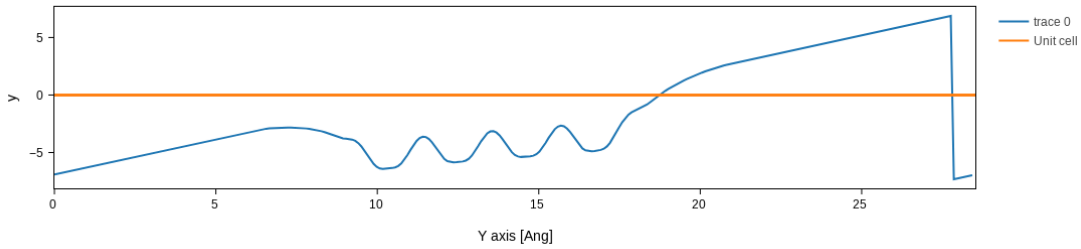
[23]:
```
E6 = sisl.get_sile("inputs6/siesta.VT").plot()
E6
```



[50]:
```
E6 = sisl.get_sile("inputs6/siesta.VT").plot(axes="yx", cmid=0)
E6
```

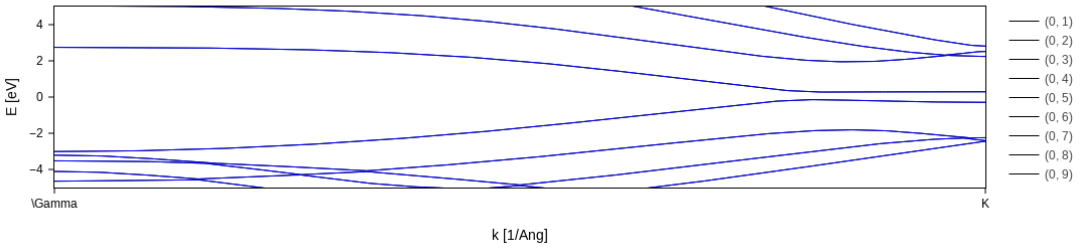


[54]:
```
E6 = sisl.get_sile("inputs6/siesta.VT").plot(axes="y", cmid=0)
E6
```

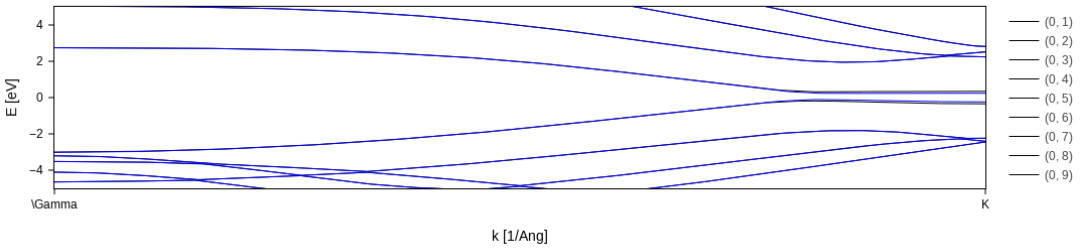


Comparem les estructures de bandes amb camp 0, 0.05 i 0.5 V/A,

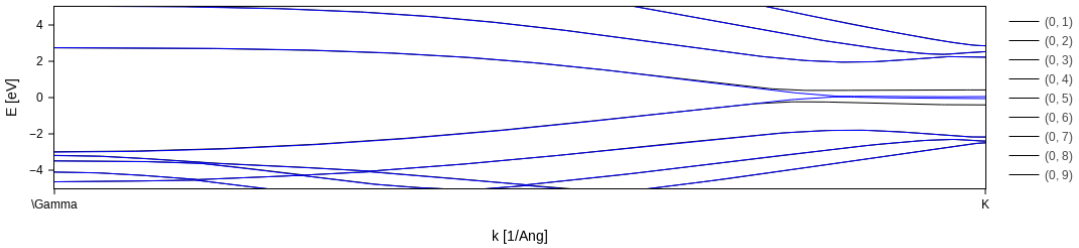
[56]:
```
bands_plot4
```



[57]:
```
bands_plot5
```



[58]:
```
bands_plot6
```


E [eV]
4
2
0
−2
−4
\Gamma
K
k [1/Ang]
(0, 1)
(0, 2)
(0, 3)
(0, 4)
(0, 5)
(0, 6)
(0, 7)
(0, 8)
(0, 9)

[ ]: