SKEO

Slater-**K**oster LCAO tight-binding modeling with **E**volutionary **O**ptimization

Load NC algebra library

Load noncommutative algebra library:

In[1]:=
```
If[Length[PacletFind["NCAlgebra"]] == 0, PacletInstall[
  "https://github.com/NCAlgebra/NC/blob/master/NCAlgebra-6.0.3.paclet?raw=true
    "]];
<< NCAlgebra`;
SetNonCommutative[s, y, z, x, xy, yz, z2, xz, x2y2];
(*when caclulating SK elements orbitals should not be commutative*)
```

o⋯ długość znajdź pakiet zainstaluj pakiet

NCAlgebra : All lower cap single letter symbols (e.g. a,b,c,...) were set as noncommutative.

Load SKEO library

In[4]:=
```
<< (NotebookDirectory[] <> "SKEO_lib.mx")
NCExpandFunc = NCExpand;(* from NCAlgebra lib *)
```

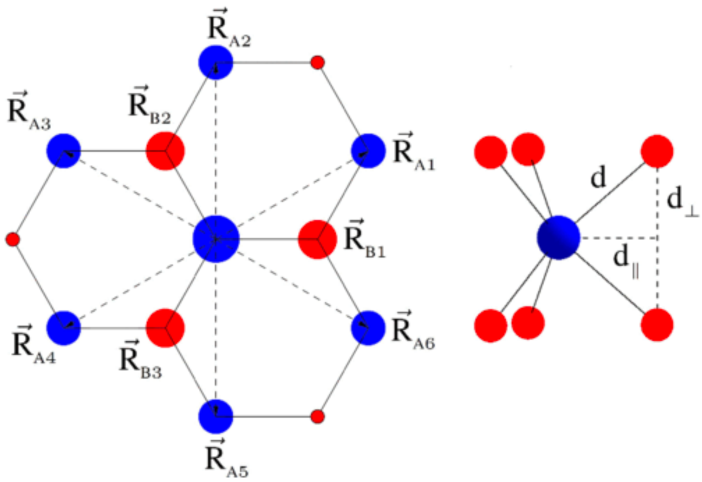
katalog notatnika

TMDC monolayer : 3-band model

TBA

TMDC monolayer: 11-band model

In this section we follow the model of $M X_2$ monolayers introduced in https://journals.aps.org/prb/abstract/10.1103/PhysRevB.97.085153



;

Now, let’s define basis orbitals (we are working in a basis of cubic harmonics: https://en.wikipedia.org/wiki/Cubic_harmonic)
Note that some of basis elements (*PE* and *PO* representing chalcogenide dimer) are composed of orbitals localized on different lattice nodes.

Basis definition

In[6]:= $Dp2 = \frac{1}{\sqrt{2}}\,(x2y2 + I\,xy)$; (*even orbital at M*)
jedność urojona

$Dp1 = \frac{-1}{\sqrt{2}}\,(xz + I\,yz)$; (*odd orbital at M*)
jedność urojona

$D0 = z2$; (*even orbital at M*)

$Dm1 = \frac{1}{\sqrt{2}}\,(xz - I\,yz)$; (*odd orbital at M*)
jedność urojona

$Dm2 = \frac{1}{\sqrt{2}}\,(x2y2 - I\,xy)$; (*even orbital at M*)
jedność urojona

$PEp1 = \left\{\frac{-1}{2}\,(x + I\,y),\ \frac{-1}{2}\,(x + I\,y)\right\}$;
jedność urojona jedność urojona

(*even X2 dimer composed of up and down orbital*)

$PE0 = \left\{\frac{1}{\sqrt{2}}\,z,\ \frac{-1}{\sqrt{2}}\,z\right\}$; (*even X2 dimer composed of up and down orbital*)

$PEm1 = \left\{\frac{1}{2}\,(x - I\,y),\ \frac{1}{2}\,(x - I\,y)\right\}$;
jedność urojona jedność urojona

(*even X2 dimer composed of up and down orbital*)

$POp1 = \left\{\frac{-1}{2}\,(x + I\,y),\ \frac{1}{2}\,(x + I\,y)\right\}$;
jedność urojona jedność urojona

(*odd X2 dimer composed of up and down orbital*)

$PO0 = \left\{\frac{1}{\sqrt{2}}\,z,\ \frac{1}{\sqrt{2}}\,z\right\}$; (*odd X2 dimer composed of up and down orbital*)

$POm1 = \left\{\frac{1}{2}\,(x - I\,y),\ \frac{1}{2}\,(-x + I\,y)\right\}$;
jedność urojona jedność urojona

(*odd X2 dimer composed of up and down orbital*);

Collect all basis elements :

In[17]:= orbitals = {Dm2, D0, Dp2, PEm1, PE0, PEp1, Dm1, Dp1, POm1, PO0, POp1};

Hoppings definition

Now define Matrix of hoppings for the each possible bond (we assume Next Nearest Neighbour approximation)

```
hopMM = {{3/2 dr, √3/2 dr, 0}, {0, √3 dr, 0}, {-3/2 dr, √3/2 dr, 0},
    {-3/2 dr, -√3/2 dr, 0}, {0, -√3 dr, 0}, {3/2 dr, -√3/2 dr, 0}};
mxu = {{dr, 0, dp}, {-1/2 dr, √3/2 dr, dp}, {-1/2 dr, -√3/2 dr, dp}};
xum = {{-dr, 0, -dp}, {1/2 dr, -√3/2 dr, -dp}, {1/2 dr, √3/2 dr, -dp}};
mxd = {{dr, 0, -dp}, {-1/2 dr, √3/2 dr, -dp}, {-1/2 dr, -√3/2 dr, -dp}};
xdm = {{-dr, 0, dp}, {1/2 dr, -√3/2 dr, dp}, {1/2 dr, √3/2 dr, dp}};
hopMX = {mxu, mxd, {1, 2}};
hopXM = {xum, xdm, {2, 1}};(* last entry, {2,1},
means that hopping is from orbital combined of two nodes to single-noded*)
hopXX = {hopMM, 0, 0, hopMM, {2, 2}};(* 0 means that we ommit given hopping;
 (2,2) means that we hop from dimer to dimer*);
```

Hoppings in our basis. Note that hoppings between dimers (consisting of orbitals at different nodes) are combined from multiple possibilities, with the option that some of them may be omitted (using “0” entry).

In our case <*up-element, down-element* | *up-element, down-element*> element has 4 possible hoppings to be defined *{<up,up>, <up,down>, <down|up>, <down|down>}*.

Here we decided to skip more distant mixed *up-down* and *down-up* hoppings.

```
In[26]:= Hop = {
    {hopMM, hopMM, hopMM, hopMX, hopMX, hopMX, 0, 0, 0, 0, 0},
    {hopMM, hopMM, hopMM, hopMX, hopMX, hopMX, 0, 0, 0, 0, 0},
    {hopMM, hopMM, hopMM, hopMX, hopMX, hopMX, 0, 0, 0, 0, 0},
    {hopXM, hopXM, hopXM, hopXX, hopXX, hopXX, 0, 0, 0, 0, 0},
    {hopXM, hopXM, hopXM, hopXX, hopXX, hopXX, 0, 0, 0, 0, 0},
    {hopXM, hopXM, hopXM, hopXX, hopXX, hopXX, 0, 0, 0, 0, 0},
    {0, 0, 0, 0, 0, 0, hopMM, hopMM, hopMX, hopMX, hopMX},
    {0, 0, 0, 0, 0, 0, hopMM, hopMM, hopMX, hopMX, hopMX},
    {0, 0, 0, 0, 0, 0, hopXM, hopXM, hopXX, hopXX, hopXX},
    {0, 0, 0, 0, 0, 0, hopXM, hopXM, hopXX, hopXX, hopXX},
    {0, 0, 0, 0, 0, 0, hopXM, hopXM, hopXX, hopXX, hopXX}};
```

We also ommit hoppings between even and odd orbitals (zeros in Hop matrix) .

Tests

Single hoppings

In[∘]:=
```
GetHoppingSingle[D0, D0, x, y, z]
```

Out[∘]=

$$\frac{3 z^2 \left(\frac{x^2}{x^2+y^2+z^2}+\frac{y^2}{x^2+y^2+z^2}\right) V_{d^2 \pi}}{x^2+y^2+z^2}+\frac{3}{4}\left(\frac{x^2}{x^2+y^2+z^2}+\frac{y^2}{x^2+y^2+z^2}\right)^2 V_{d^2 \delta}+\left(\frac{z^2}{x^2+y^2+z^2}+\frac{1}{2}\left(-\frac{x^2}{x^2+y^2+z^2}-\frac{y^2}{x^2+y^2+z^2}\right)\right)^2 V_{d^2 \sigma}$$

In[∘]:=
```
FullSimplify[GetHopping[Dm1, P0p1,
  {{{dr, 0, dp}}, {{dr, 0, -dp}}, {1, 2}}, True] /. {dp^2 + dr^2 → d^2}]
```
uprość pełniej · prawda

Out[∘]=

$$-\frac{dp\, dr^2\, e^{i\, dr\, kx} \left(2 V_{d p \pi}-\sqrt{3}\, V_{d p \sigma}\right)}{\sqrt{2}\, \left(d^2\right)^{3/2}}$$

In[∘]:=

$$\text{FullSimplify}\left[\text{GetHopping}\left[\text{Dm2, D0, } \left\{\left\{\frac{3}{2}\text{ dr, } \frac{\sqrt{3}}{2}\text{ dr, } 0\right\}\right\}\text{, True}\right]\right]$$

uprość pełniej · prawda

Out[∘]=

$$\frac{\left(3 i+\sqrt{3}\right) e^{\frac{1}{2} i\, dr\, \left(3 kx+\sqrt{3}\, ky\right)} \left(V_{d^2 \delta}-V_{d^2 \sigma}\right)}{8 \sqrt{2}}$$

Matrix elements

In[∘]:=
```
H1v1 = FullSimplify[GetHopping[D0, D0, hopMM, True]]
```
uprość pełniej · prawda

Out[∘]=

$$\frac{1}{2}\left(\text{Cos}\left[\sqrt{3}\text{ dr ky}\right]+\text{Cos}\left[\frac{1}{2}\text{ dr }\left(3\text{ kx}-\sqrt{3}\text{ ky}\right)\right]+\text{Cos}\left[\frac{1}{2}\text{ dr }\left(3\text{ kx}+\sqrt{3}\text{ ky}\right)\right]\right)\left(3 V_{d^2 \delta}+V_{d^2 \sigma}\right)$$

In[∘]:=

$$\text{FullSimplify}\left[\text{H1v1} == \frac{1}{2}\left(3 V_{d^2 \delta}+V_{d^2 \sigma}\right)\left(2\,\text{Cos}[3/2\text{ kx dr}] * \text{Cos}\left[\sqrt{3}\Big/2\text{ ky dr}\right]+\text{Cos}\left[\sqrt{3}\text{ ky dr}\right]\right)\right]$$

uprość pełniej · cosinus · cosinus · cosinus

Out[∘]=
```
True
```

In[∘]:=
```
H1v2 = FullSimplify[GetHopping[Dm2, D0, hopMM, True]]
```
uprość pełniej   prawda

Out[∘]=

$$\frac{1}{4}\sqrt{\frac{3}{2}}\left(-2\,\text{Cos}\left[\sqrt{3}\ \text{dr ky}\right]+\left(1-\mathrm{i}\sqrt{3}\right)\text{Cos}\left[\frac{1}{2}\,\text{dr}\left(3\,\text{kx}-\sqrt{3}\ \text{ky}\right)\right]+\left(1+\mathrm{i}\sqrt{3}\right)\text{Cos}\left[\frac{1}{2}\,\text{dr}\left(3\,\text{kx}+\sqrt{3}\ \text{ky}\right)\right]\right)\left(V_{d^2\,\delta}-V_{d^2\,\sigma}\right)$$

In[∘]:=
$$\text{FullSimplify}\left[\text{H1v2} == \frac{-\sqrt{3}}{2\sqrt{2}}\left(V_{d^2\,\sigma}-V_{d^2\,\delta}\right)\left(\text{Cos}\left[3/2\ \text{kx dr}+\sqrt{3}\Big/2\ \text{ky dr}\right]\text{Exp}[\text{I Pi}/3]+\text{Cos}\left[3/2\ \text{kx dr}-\sqrt{3}\Big/2\ \text{ky dr}\right]\text{Exp}[-\text{I Pi}/3]-\text{Cos}\left[\sqrt{3}\ \text{ky dr}\right]\right)\right]$$
uprość pełniej   cosinus   fu··· · pi   cosinus   funkc·· · pi   cosinus

Out[∘]=
```
True
```

In[∘]:=
```
H5v5 = FullSimplify[GetHopping[PE0, PE0, hopXX, True]]
```
uprość pełniej   prawda

Out[∘]=

$$2\left(\text{Cos}\left[\sqrt{3}\ \text{dr ky}\right]+\text{Cos}\left[\frac{1}{2}\,\text{dr}\left(3\,\text{kx}-\sqrt{3}\ \text{ky}\right)\right]+\text{Cos}\left[\frac{1}{2}\,\text{dr}\left(3\,\text{kx}+\sqrt{3}\ \text{ky}\right)\right]\right)V_{p^2\,\pi}$$

In[∘]:=
$$\text{FullSimplify}\left[\text{H5v5} == V_{p^2\,\pi}\left(4\,\text{Cos}[3/2\ \text{kx dr}]*\text{Cos}\left[\sqrt{3}\Big/2\ \text{ky dr}\right]+2\,\text{Cos}\left[\sqrt{3}\ \text{ky dr}\right]\right)\right]$$
uprość pełniej   cosinus   cosinus   cosinus

Out[∘]=
```
True
```

In[∘]:=
```
H4v6 = FullSimplify[GetHopping[PEm1, PEp1, hopXX, True]]
```
uprość pełniej   prawda

Out[∘]=

$$\frac{1}{2}\left(-2\,\text{Cos}\left[\sqrt{3}\ \text{dr ky}\right]+\left(1-\mathrm{i}\sqrt{3}\right)\text{Cos}\left[\frac{1}{2}\,\text{dr}\left(3\,\text{kx}-\sqrt{3}\ \text{ky}\right)\right]+\left(1+\mathrm{i}\sqrt{3}\right)\text{Cos}\left[\frac{1}{2}\,\text{dr}\left(3\,\text{kx}+\sqrt{3}\ \text{ky}\right)\right]\right)\left(V_{p^2\,\pi}-V_{p^2\,\sigma}\right)$$

In[∘]:=
$$\text{FullSimplify}\left[\text{H4v6} == \left(V_{p^2\,\sigma}-V_{p^2\,\pi}\right)\left(\text{Cos}\left[3/2\ \text{kx dr}+\sqrt{3}\Big/2\ \text{ky dr}\right]\text{Exp}[\text{I Pi}/3]+\text{Cos}\left[3/2\ \text{kx dr}-\sqrt{3}\Big/2\ \text{ky dr}\right]\text{Exp}[-\text{I Pi}/3]-\text{Cos}\left[\sqrt{3}\ \text{ky dr}\right]\right)*(-1)\right]$$
uprość pełniej   cosinus   fu··· · pi   cosinus   funkc·· · pi   cosinus

Out[∘]=
```
True
```

In[∘]:=
$$\text{H3v6} = \text{FullSimplify}\left[\text{GetHopping}[\text{Dp2}, \text{PEp1}, \text{hopMX}, \text{True}]\ /.\ \left\{\text{dp}^2+\text{dr}^2\to \text{d}^2\right\}\right]$$
uprość pełniej   prawda

Out[∘]=

$$\frac{1}{4\sqrt{2}\left(\text{d}^2\right)^{3/2}}\,e^{-\frac{1}{2}\mathrm{i}\,\text{dr}\left(\text{kx}+\sqrt{3}\ \text{ky}\right)}\left(2\,\text{dr}\left(-2\,\text{d}^2+\text{dr}^2\right)\left(1-\mathrm{i}\sqrt{3}+\left(1+\mathrm{i}\sqrt{3}\right)e^{\mathrm{i}\sqrt{3}\ \text{dr ky}}-2\,e^{\frac{1}{2}\mathrm{i}\,\text{dr}\left(3\,\text{kx}+\sqrt{3}\ \text{ky}\right)}\right)V_{d\,p\,\pi}-\text{dr}^3\left(-3\,\mathrm{i}+\sqrt{3}+\left(3\,\mathrm{i}+\sqrt{3}\right)e^{\mathrm{i}\sqrt{3}\ \text{dr ky}}-2\sqrt{3}\,e^{\frac{1}{2}\mathrm{i}\,\text{dr}\left(3\,\text{kx}+\sqrt{3}\ \text{ky}\right)}\right)V_{d\,p\,\sigma}\right)$$

In[ ]:=
```
FullSimplify[H3v6 == dr/(Sqrt[2] d) (Sqrt[3] / 2 Vdpσ (dp^2 / d^2 - 1) - Vdpπ (dp^2 / d^2 + 1))
 (Exp[I kx dr] + Exp[-I kx dr / 2 + I Sqrt[3] ky dr / 2 - 2 I Pi / 3] +
   Exp[-I kx dr / 2 - I Sqrt[3] ky dr / 2 + 2 I Pi / 3]) * (-1)]
uprość pełniej
fu··· jedność ur·· funkc·· jedność urojona jedność urojona · pi
funkc·· jedność urojona jedność urojona · pi
```

Out[ ]=

$$\frac{1}{\sqrt{d^2}}\, d\, dr\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \Big(2 \left(-2 d^3 + \sqrt{d^2}\, (d^2 + dp^2) + d\, dr^2\right) \left(-1 + i \sqrt{3} + (-1 - i \sqrt{3})\, e^{i \sqrt{3}\, dr\, ky} + 2\, e^{\frac{1}{2} i\, dr\, (3 kx + \sqrt{3}\, ky)}\right) V_{dp\pi} - \left((d^2)^{3/2} - \sqrt{d^2}\, dp^2 - d\, dr^2\right) \left(-3 i + \sqrt{3} + (3 i + \sqrt{3})\, e^{i \sqrt{3}\, dr\, ky} - 2 \sqrt{3}\, e^{\frac{1}{2} i\, dr\, (3 kx + \sqrt{3}\, ky)}\right) V_{dp\sigma}\Big) == 0$$

In[ ]:=
```
H7v11 = FullSimplify[GetHopping[Dm1, POp1, hopMX, True] /. {dp^2 + dr^2 → d^2}]
        uprość pełniej                              prawda
```

Out[ ]=

$$\frac{1}{2 \sqrt{2}\, (d^2)^{3/2}}\, dp\, dr^2\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \Big(2 \left(1 - i \sqrt{3} + (1 + i \sqrt{3})\, e^{i \sqrt{3}\, dr\, ky} - 2\, e^{\frac{1}{2} i\, dr\, (3 kx + \sqrt{3}\, ky)}\right) V_{dp\pi} - \left(-3 i + \sqrt{3} + (3 i + \sqrt{3})\, e^{i \sqrt{3}\, dr\, ky} - 2 \sqrt{3}\, e^{\frac{1}{2} i\, dr\, (3 kx + \sqrt{3}\, ky)}\right) V_{dp\sigma}\Big)$$

In[ ]:=
```
FullSimplify[H7v11 == - dp dr^2/(Sqrt[2] d^3) (Sqrt[3] Vdpσ - 2 Vdpπ)
 (Exp[I kx dr] + Exp[-I kx dr / 2 + I Sqrt[3] ky dr / 2 - 2 I Pi / 3] +
   Exp[-I kx dr / 2 - I Sqrt[3] ky dr / 2 + 2 I Pi / 3]) * (-1)]
uprość pełniej
fu··· jedność ur·· funkc·· jedność urojona jedność urojona · pi
funkc·· jedność urojona jedność urojona · pi
```

Out[ ]=

$$\frac{1}{d \sqrt{d^2}} \left(-d + \sqrt{d^2}\right) dp\, dr\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \Big(\left(-2 + 2 i \sqrt{3} + (-2 - 2 i \sqrt{3})\, e^{i \sqrt{3}\, dr\, ky} + 4\, e^{\frac{1}{2} i\, dr\, (3 kx + \sqrt{3}\, ky)}\right) V_{dp\pi} + \left(-3 i + \sqrt{3} + (3 i + \sqrt{3})\, e^{i \sqrt{3}\, dr\, ky} - 2 \sqrt{3}\, e^{\frac{1}{2} i\, dr\, (3 kx + \sqrt{3}\, ky)}\right) V_{dp\sigma}\Big) == 0$$

In[∘]:=

```
H7v10 = FullSimplify[GetHopping[Dm1, P00, hopMX, True] /. {dp^2 + dr^2 → d^2}]
```

uprość pełniej · prawda

Out[∘]=

$$\frac{1}{2\,(d^2)^{3/2}} dr\, e^{-\frac{1}{2} i\, dr\,(kx+\sqrt{3}\,ky)} \Big(\big(d^2-2\,dp^2\big)\Big(1+i\sqrt{3}+\big(1-i\sqrt{3}\big)\,e^{i\sqrt{3}\,dr\,ky}-2\,e^{\frac{1}{2} i\,dr\,(3\,kx+\sqrt{3}\,ky)}\Big)V_{dp\pi}+ dp^2\Big(3\,i+\sqrt{3}+\big(-3\,i+\sqrt{3}\big)\,e^{i\sqrt{3}\,dr\,ky}-2\sqrt{3}\,e^{\frac{1}{2} i\,dr\,(3\,kx+\sqrt{3}\,ky)}\Big)V_{dp\sigma}\Big)$$

In[∘]:=

```
FullSimplify[H7v10 == -dr/d (dp^2/d^2 (√3 Vdpσ - 2 Vdpπ) + Vdpπ)
  (Exp[I kx dr] + Exp[-I kx dr / 2 + I √3 ky dr / 2 + 2 I Pi / 3] +
   Exp[-I kx dr / 2 - I √3 ky dr / 2 - 2 I Pi / 3])]
```

uprość pełniej · funkcja · jedność urojona · funkcja · jedność urojona · jedność urojona · pi · funkcja · jedność urojona · jedność urojona · pi

Out[∘]=

$$\frac{1}{\sqrt{d^2}}\, d\,\big(-d+\sqrt{d^2}\big)\, dr\, e^{-\frac{1}{2} i\,dr\,(kx+\sqrt{3}\,ky)} \Big(\big(d^2-2\,dp^2\big)\Big(-1-i\sqrt{3}+i\,\big(i+\sqrt{3}\big)\,e^{i\sqrt{3}\,dr\,ky}+2\,e^{\frac{1}{2} i\,dr\,(3\,kx+\sqrt{3}\,ky)}\Big)V_{dp\pi}- dp^2\Big(3\,i+\sqrt{3}+\big(-3\,i+\sqrt{3}\big)\,e^{i\sqrt{3}\,dr\,ky}-2\sqrt{3}\,e^{\frac{1}{2} i\,dr\,(3\,kx+\sqrt{3}\,ky)}\Big)V_{dp\sigma}\Big) == 0$$

In[∘]:=

```
H8v9 = FullSimplify[GetHopping[Dp1, P0m1, hopMX, True] /. {dp^2 + dr^2 → d^2}]
```

uprość pełniej · prawda

Out[∘]=

$$\frac{1}{2\sqrt{2}\,(d^2)^{3/2}} dp\, dr^2\, e^{-\frac{1}{2} i\,dr\,(kx+\sqrt{3}\,ky)} \Big(2\Big(1+i\sqrt{3}+\big(1-i\sqrt{3}\big)\,e^{i\sqrt{3}\,dr\,ky}-2\,e^{\frac{1}{2} i\,dr\,(3\,kx+\sqrt{3}\,ky)}\Big)V_{dp\pi}- \Big(3\,i+\sqrt{3}+\big(-3\,i+\sqrt{3}\big)\,e^{i\sqrt{3}\,dr\,ky}-2\sqrt{3}\,e^{\frac{1}{2} i\,dr\,(3\,kx+\sqrt{3}\,ky)}\Big)V_{dp\sigma}\Big)$$

In[∘]:=

```
FullSimplify[H8v9 ==
  dp dr^2/(√2 d^3) (√3 Vdpσ - 2 Vdpπ) (Exp[I kx dr] + Exp[-I kx dr / 2 + I √3 ky dr / 2 + 2 I Pi / 3] +
   Exp[-I kx dr / 2 - I √3 ky dr / 2 - 2 I Pi / 3])]
```

uprość pełniej · funkcja · jedność urojona · funkcja · jedność urojona · jedność urojona · pi · funkcja · jedność urojona · jedność urojona · pi

Out[∘]=

$$\frac{1}{d\sqrt{d^2}}\big(-d+\sqrt{d^2}\big)\, dp\, dr\, e^{-\frac{1}{2} i\,dr\,(kx+\sqrt{3}\,ky)} \Big(\Big(-2-2\,i\sqrt{3}+2\,i\,\big(i+\sqrt{3}\big)\,e^{i\sqrt{3}\,dr\,ky}+4\,e^{\frac{1}{2} i\,dr\,(3\,kx+\sqrt{3}\,ky)}\Big)V_{dp\pi}+ \Big(3\,i+\sqrt{3}+\big(-3\,i+\sqrt{3}\big)\,e^{i\sqrt{3}\,dr\,ky}-2\sqrt{3}\,e^{\frac{1}{2} i\,dr\,(3\,kx+\sqrt{3}\,ky)}\Big)V_{dp\sigma}\Big) == 0$$

In[ ]:=
```
H8v10 = FullSimplify[GetHopping[Dp1, P00, hopMX, True] /. {dp^2 + dr^2 → d^2}]
```
Out[ ]=
$$\frac{1}{2\,(d^2)^{3/2}}\,dr\,e^{-\frac{1}{2}i\,dr\,(kx+\sqrt{3}\,ky)}\Big(\big(d^2-2\,dp^2\big)\big(-1+i\sqrt{3}+(-1-i\sqrt{3})\,e^{i\sqrt{3}\,dr\,ky}+2\,e^{\frac{1}{2}i\,dr\,(3\,kx+\sqrt{3}\,ky)}\big)\,V_{dp\pi}-dp^2\big(-3\,i+\sqrt{3}+(3\,i+\sqrt{3})\,e^{i\sqrt{3}\,dr\,ky}-2\sqrt{3}\,e^{\frac{1}{2}i\,dr\,(3\,kx+\sqrt{3}\,ky)}\big)\,V_{dp\sigma}\Big)$$

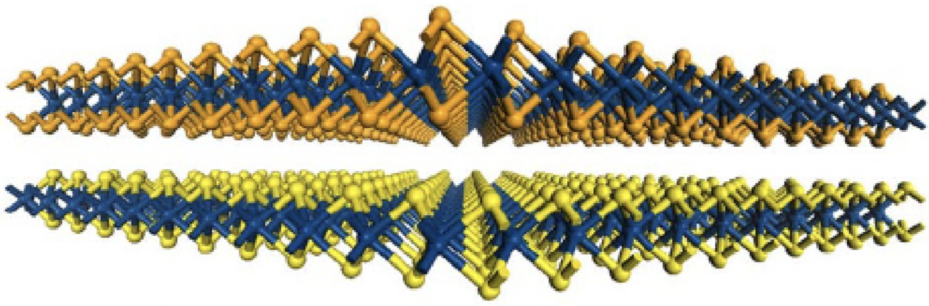
In[ ]:=
```
FullSimplify[H8v10 == dr/d (dp^2/d^2 (Sqrt[3] V_dpσ - 2 V_dpπ) + V_dpπ)
  (Exp[I kx dr] + Exp[-I kx dr / 2 + I Sqrt[3] ky dr / 2 - 2 I Pi / 3] +
    Exp[-I kx dr / 2 - I Sqrt[3] ky dr / 2 + 2 I Pi / 3])]
```
Out[ ]=
$$\frac{1}{\sqrt{d^2}}\,d\,\big(-d+\sqrt{d^2}\big)\,dr\,e^{-\frac{1}{2}i\,dr\,(kx+\sqrt{3}\,ky)}\Big(\big(d^2-2\,dp^2\big)\big(-1+i\sqrt{3}+(-1-i\sqrt{3})\,e^{i\sqrt{3}\,dr\,ky}+2\,e^{\frac{1}{2}i\,dr\,(3\,kx+\sqrt{3}\,ky)}\big)\,V_{dp\pi}-dp^2\big(-3\,i+\sqrt{3}+(3\,i+\sqrt{3})\,e^{i\sqrt{3}\,dr\,ky}-2\sqrt{3}\,e^{\frac{1}{2}i\,dr\,(3\,kx+\sqrt{3}\,ky)}\big)\,V_{dp\sigma}\Big)=0$$

In[ ]:=
```
H9v11 = FullSimplify[GetHopping[POm1, POp1, hopXX, True] /. {dp^2 + dr^2 → d^2}]
```
Out[ ]=
$$\frac{1}{2}\Big(-2\,\mathrm{Cos}\big[\sqrt{3}\,dr\,ky\big]+(1-i\sqrt{3})\,\mathrm{Cos}\Big[\frac{1}{2}\,dr\,(3\,kx-\sqrt{3}\,ky)\Big]+(1+i\sqrt{3})\,\mathrm{Cos}\Big[\frac{1}{2}\,dr\,(3\,kx+\sqrt{3}\,ky)\Big]\Big)\big(V_{p^2\pi}-V_{p^2\sigma}\big)$$

In[ ]:=
```
FullSimplify[H9v11 == (V_p²σ - V_p²π) (Cos[3/2 kx dr + Sqrt[3]/2 ky dr] Exp[I Pi/3] +
    Cos[3/2 kx dr - Sqrt[3]/2 ky dr] Exp[-I Pi/3] - Cos[Sqrt[3] ky dr]) * (-1)]
```
Out[ ]=
```
True
```
In[ ]:=
```
H9v10 = FullSimplify[GetHopping[POm1, P00, hopXX, True] /. {dp^2 + dr^2 → d^2}]
```
Out[ ]=
```
0
```

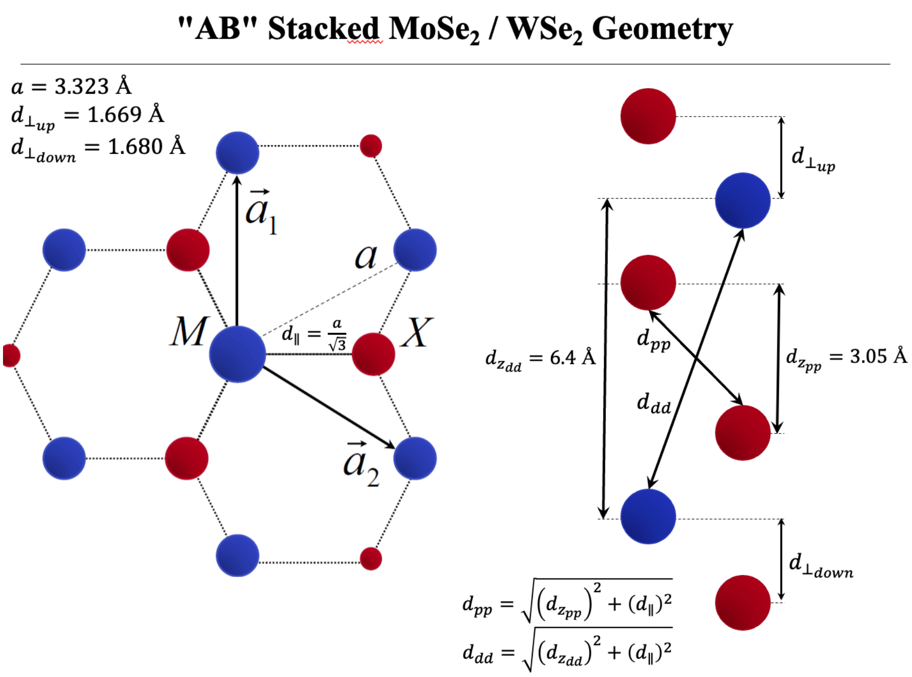
TMDC heterostructure

In this section we introduce TB model for stacked TMDC heterostructure.



;

Interalyer hoppings



;

Let' s define interalyer hoppings <top layer | bottom layer> (intralayer are the same as in the previous chapter):

In[27]:=
```
ihopMM = List[{-dr, 0, -dzdd}, {1/2 dr, -Sqrt[3]/2 dr, -dzdd}, {1/2 dr, Sqrt[3]/2 dr, -dzdd}];

ihopMX = {{{0, 0, -dzdp}}, 0, {1, 2}};
(* M from top layer only coupled with (nearer) up X-atom from bottom layer *)
ihopXM = {0, {{0, 0, -dzdp}}, {2, 1}}; (* only (nearer) down X-
 atom from top layer is coupled with M atom from bottom layer *)

ihopxx = List[{dr, 0, -dzpp}, {-1/2 dr, Sqrt[3]/2 dr, -dzpp}, {-1/2 dr, -Sqrt[3]/2 dr, -dzpp}];

ihopXX = {0, 0, ihopxx, 0, {2, 2}};(* only down X-
 atom from top dimer is coupled with up X-atom from bottom dimer *)
```

In[32]:=
```
IHop = {
    {ihopMM, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopMM, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopMM, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopXM, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX},
    {ihopXM, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX},
    {ihopXM, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX}};
```

In[33]:=
```
Iorbitals = {Dm2, D0, Dp2, PEm1, PE0, PEp1};
```

In[34]:=
```
HSKinter = HSKHoppings[Iorbitals, IHop, True];
```

prawda

[1,1]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2} e^{-\frac{1}{2} i\, dr\,\left(2\,kx+\sqrt{3}\,ky\right)} \left(e^{\frac{3\,i\,dr\,kx}{2}}+e^{\frac{1}{2} i \sqrt{3}\,dr\,ky}+e^{\frac{1}{2} i\, dr\,\left(3\,kx+2\sqrt{3}\,ky\right)}\right) \left(4\left(dr^4+2\,dr^2\,dzdd^2\right) V_{d^2\,\pi}+\left(dr^4+8\,dr^2\,dzdd^2+8\,dzdd^4\right) V_{d^2\,\delta}+3\,dr^4\,V_{d^2\,\sigma}\right)$$

[1,2]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2} \sqrt{\frac{3}{2}}\,dr^2\,e^{-\frac{1}{2} i\, dr\,\left(2\,kx+\sqrt{3}\,ky\right)} \left(\left(-1-i\sqrt{3}\right) e^{\frac{3\,i\,dr\,kx}{2}}+2\,e^{\frac{1}{2} i \sqrt{3}\,dr\,ky}+i\left(i+\sqrt{3}\right) e^{\frac{1}{2} i\, dr\,\left(3\,kx+2\sqrt{3}\,ky\right)}\right) \left(-4\,dzdd^2\,V_{d^2\,\pi}+\left(dr^2+2\,dzdd^2\right) V_{d^2\,\delta}-\left(dr^2-2\,dzdd^2\right) V_{d^2\,\sigma}\right)$$

[1,3]

$$\frac{1}{16\left(dr^2+dzdd^2\right)^2} dr^4\,e^{-\frac{1}{2} i\, dr\,\left(2\,kx+\sqrt{3}\,ky\right)} \left(\left(1-i\sqrt{3}\right) e^{\frac{3\,i\,dr\,kx}{2}}-2\,e^{\frac{1}{2} i \sqrt{3}\,dr\,ky}+\left(1+i\sqrt{3}\right) e^{\frac{1}{2} i\, dr\,\left(3\,kx+2\sqrt{3}\,ky\right)}\right) \left(4\,V_{d^2\,\pi}-V_{d^2\,\delta}-3\,V_{d^2\,\sigma}\right)$$

[1,4]

0

[1,5]

0

[1,6]

0

[2,1]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2} \sqrt{\frac{3}{2}}\,dr^2\,e^{-\frac{1}{2} i\, dr\,\left(2\,kx+\sqrt{3}\,ky\right)} \left(i\left(i+\sqrt{3}\right) e^{\frac{3\,i\,dr\,kx}{2}}+2\,e^{\frac{1}{2} i \sqrt{3}\,dr\,ky}+\left(-1-i\sqrt{3}\right) e^{\frac{1}{2} i\, dr\,\left(3\,kx+2\sqrt{3}\,ky\right)}\right) \left(-4\,dzdd^2\,V_{d^2\,\pi}+\left(dr^2+2\,dzdd^2\right) V_{d^2\,\delta}-\left(dr^2-2\,dzdd^2\right) V_{d^2\,\sigma}\right)$$

[2,2]

$$\frac{1}{4\left(dr^2+dzdd^2\right)^2} e^{-\frac{1}{2} i\, dr\,\left(2\,kx+\sqrt{3}\,ky\right)} \left(e^{\frac{3\,i\,dr\,kx}{2}}+e^{\frac{1}{2} i \sqrt{3}\,dr\,ky}+e^{\frac{1}{2} i\, dr\,\left(3\,kx+2\sqrt{3}\,ky\right)}\right) \left(12\,dr^2\,dzdd^2\,V_{d^2\,\pi}+3\,dr^4\,V_{d^2\,\delta}+\left(dr^2-2\,dzdd^2\right)^2 V_{d^2\,\sigma}\right)$$

[2,3]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2}\sqrt{\frac{3}{2}}\,dr^2\,e^{-\frac{1}{2}\,i\,dr\,\left(2\,kx+\sqrt{3}\,ky\right)}\left(\left(-1-i\sqrt{3}\right)e^{\frac{3\,i\,dr\,kx}{2}}+2\,e^{\frac{1}{2}\,i\,\sqrt{3}\,dr\,ky}+i\left(i+\sqrt{3}\right)e^{\frac{1}{2}\,i\,dr\,\left(3\,kx+2\,\sqrt{3}\,ky\right)}\right)\left(-4\,dzdd^2\,V_{d^2\,\pi}+\left(dr^2+2\,dzdd^2\right)V_{d^2\,\delta}-\left(dr^2-2\,dzdd^2\right)V_{d^2\,\sigma}\right)$$

[2,4]
0

[2,5]

$$\frac{dzdp\,V_{d\,p\,\sigma}}{\sqrt{2}\,\sqrt{dzdp^2}}$$

[2,6]
0

[3,1]

$$\frac{1}{16\left(dr^2+dzdd^2\right)^2}dr^4\,e^{-\frac{1}{2}\,i\,dr\,\left(2\,kx+\sqrt{3}\,ky\right)}\left(\left(1+i\sqrt{3}\right)e^{\frac{3\,i\,dr\,kx}{2}}-2\,e^{\frac{1}{2}\,i\,\sqrt{3}\,dr\,ky}+\left(1-i\sqrt{3}\right)e^{\frac{1}{2}\,i\,dr\,\left(3\,kx+2\,\sqrt{3}\,ky\right)}\right)\left(4\,V_{d^2\,\pi}-V_{d^2\,\delta}-3\,V_{d^2\,\sigma}\right)$$

[3,2]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2}\sqrt{\frac{3}{2}}\,dr^2\,e^{-\frac{1}{2}\,i\,dr\,\left(2\,kx+\sqrt{3}\,ky\right)}\left(i\left(i+\sqrt{3}\right)e^{\frac{3\,i\,dr\,kx}{2}}+2\,e^{\frac{1}{2}\,i\,\sqrt{3}\,dr\,ky}+\left(-1-i\sqrt{3}\right)e^{\frac{1}{2}\,i\,dr\,\left(3\,kx+2\,\sqrt{3}\,ky\right)}\right)\left(-4\,dzdd^2\,V_{d^2\,\pi}+\left(dr^2+2\,dzdd^2\right)V_{d^2\,\delta}-\left(dr^2-2\,dzdd^2\right)V_{d^2\,\sigma}\right)$$

[3,3]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2}e^{-\frac{1}{2}\,i\,dr\,\left(2\,kx+\sqrt{3}\,ky\right)}\left(e^{\frac{3\,i\,dr\,kx}{2}}+e^{\frac{1}{2}\,i\,\sqrt{3}\,dr\,ky}+e^{\frac{1}{2}\,i\,dr\,\left(3\,kx+2\,\sqrt{3}\,ky\right)}\right)\left(4\left(dr^4+2\,dr^2\,dzdd^2\right)V_{d^2\,\pi}+\left(dr^4+8\,dr^2\,dzdd^2+8\,dzdd^4\right)V_{d^2\,\delta}+3\,dr^4\,V_{d^2\,\sigma}\right)$$

[3,4]
0

[3,5]
0

[3,6]
0

[4,1]
0

[4,2]
0

[4,3]
0

[4,4]

$$\frac{e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1 + e^{i \sqrt{3}\, dr\, ky} + e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(\left(dr^2 + 2\, dzpp^2\right) V_{p^2 \pi} + dr^2\, V_{p^2 \sigma}\right)}{4 \left(dr^2 + dzpp^2\right)}$$

[4,5]

$$\frac{dr\, dzpp\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(-1 - i \sqrt{3} + i \left(i + \sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky} + 2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2 \pi} - V_{p^2 \sigma}\right)}{4 \sqrt{2} \left(dr^2 + dzpp^2\right)}$$

[4,6]

$$\frac{dr^2\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(-1 + i \sqrt{3} + \left(-1 - i \sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky} + 2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2 \pi} - V_{p^2 \sigma}\right)}{8 \left(dr^2 + dzpp^2\right)}$$

[5,1]

0

[5,2]

$$\frac{dzdp\, V_{d p \sigma}}{\sqrt{2} \sqrt{dzdp^2}}$$

[5,3]

0

[5,4]

$$\frac{dr\, dzpp\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1 - i \sqrt{3} + \left(1 + i \sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky} - 2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2 \pi} - V_{p^2 \sigma}\right)}{4 \sqrt{2} \left(dr^2 + dzpp^2\right)}$$

[5,5]

$$-\frac{e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1 + e^{i \sqrt{3}\, dr\, ky} + e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(dr^2\, V_{p^2 \pi} + dzpp^2\, V_{p^2 \sigma}\right)}{2 \left(dr^2 + dzpp^2\right)}$$

[5,6]

$$\frac{dr\, dzpp\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(-1 - i \sqrt{3} + i \left(i + \sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky} + 2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2 \pi} - V_{p^2 \sigma}\right)}{4 \sqrt{2} \left(dr^2 + dzpp^2\right)}$$

[6,1]

0

[6,2]

0

[6,3]

0

[6,4]

$$\frac{dr^2\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(-1 - i \sqrt{3} + i \left(i + \sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky} + 2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2 \pi} - V_{p^2 \sigma}\right)}{8 \left(dr^2 + dzpp^2\right)}$$

[6,5]

$$\frac{dr\, dzpp\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1 - i \sqrt{3} + \left(1 + i \sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky} - 2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2\,\pi} - V_{p^2\,\sigma}\right)}{4 \sqrt{2} \left(dr^2 + dzpp^2\right)}$$

[6,6]

$$\frac{e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1 + e^{i \sqrt{3}\, dr\, ky} + e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(\left(dr^2 + 2\, dzpp^2\right) V_{p^2\,\pi} + dr^2\, V_{p^2\,\sigma}\right)}{4 \left(dr^2 + dzpp^2\right)}$$

In[ ]:=

```
HSKinter[[2, 2]] (*D0-D0*)
```

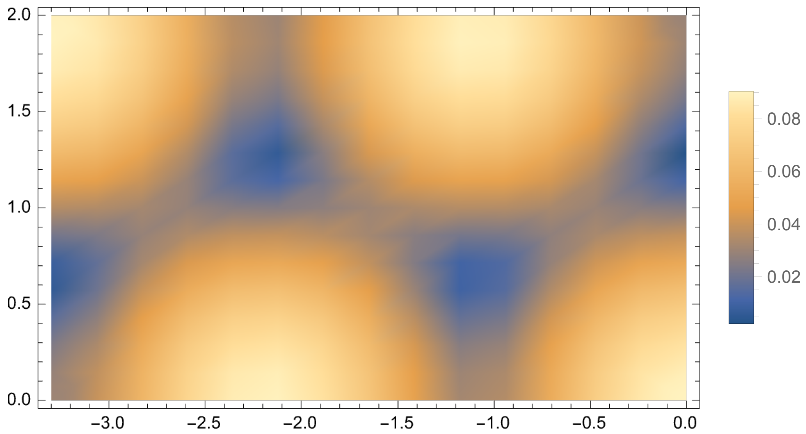
Out[ ]=

$$\frac{1}{4 \left(dr^2 + dzdd^2\right)^2} e^{-\frac{1}{2} i\, dr\, (2\, kx+\sqrt{3}\, ky)} \left(e^{\frac{3\, i\, dr\, kx}{2}} + e^{\frac{1}{2} i \sqrt{3}\, dr\, ky} + e^{\frac{1}{2} i\, dr\, (3\, kx+2 \sqrt{3}\, ky)}\right)$$
$$\left(12\, dr^2\, dzdd^2\, V_{d^2\,\pi} + 3\, dr^4\, V_{d^2\,\delta} + \left(dr^2 - 2\, dzdd^2\right)^2 V_{d^2\,\sigma}\right)$$

In[56]:=

```
DensityPlot[
wykres gęstości
 Abs[HSKinter[[2, 2]] /. {dr → 3.323 / √3 , dzpp → 3.05, dzdd → 6.4, Vd²π → 1.8318,
 wartość bezwzględna
    Vd²δ → -0.3299, Vd²σ → -0.5, Vp²π → -0.1547, Vp²σ → -1.1006}],
 {kx, -3.3, 0}, {ky, 0, 2.}, PlotLegends → Automatic, AspectRatio → Equal]
                             legenda dla grafik  automatyczny  format obrazu  równe
```

Out[56]=



In[ ]:=

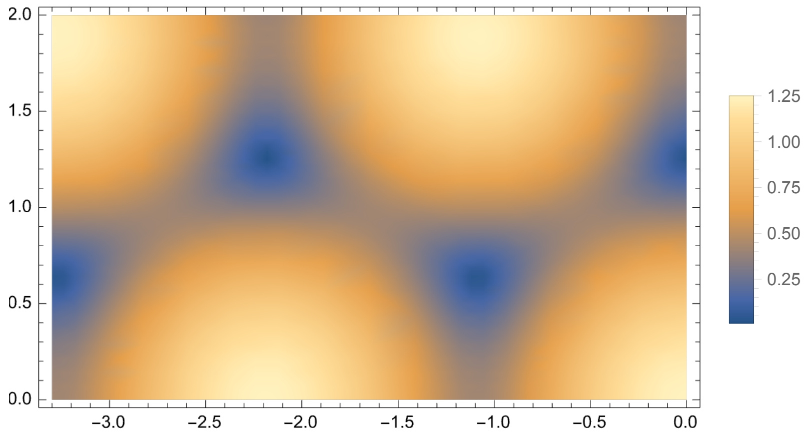
```
HSKinter[[5, 5]] (*P0-P0*)
```

Out[ ]=

$$-\frac{e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1 + e^{i \sqrt{3}\, dr\, ky} + e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(dr^2\, V_{p^2\,\pi} + dzpp^2\, V_{p^2\,\sigma}\right)}{2 \left(dr^2 + dzpp^2\right)}$$

In[55]:=
```
DensityPlot[
Abs[HSKinter[[5, 5]] /. {dr → 3.323 / √3, dzpp → 3.05, dzdd → 6.4, V_{d² π} → 1.8318,
    V_{d² δ} → -0.3299, V_{d² σ} → -0.5, V_{p² π} → -0.1547, V_{p² σ} → -1.1006}],
{kx, -3.3, 0}, {ky, 0, 2.0}, PlotLegends → Automatic, AspectRatio → Equal]
```
wykres gęstości; wartość bezwzględna; legenda dla grafik; automatyczny; format obrazu; równe

Out[55]=

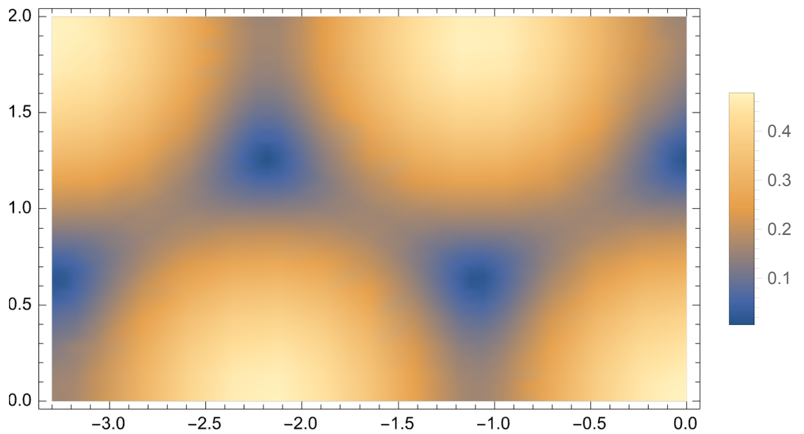


In[ ]:=
```
Abs[HSKinter[[2, 5]] /. {dr → 3.323 / √3, dzpp → 3.05, dzdd → 6.4, dzdp → 4.5,
   V_{d² π} → 1.8318, V_{d² δ} → -0.3299, V_{d² σ} → -0.5, V_{p² π} → -0.1547, V_{p² σ} → -1.1006}]
```
wartość bezwzględna

Out[ ]=
```
0.707107 Abs[V_{d p σ}]
```

In[57]:=
```
DensityPlot[
Abs[HSKinter[[1, 1]] /. {dr → 3.323 / √3, dzpp → 3.05, dzdd → 6.4, V_{d² π} → 1.8318,
    V_{d² δ} → -0.3299, V_{d² σ} → -0.5, V_{p² π} → -0.1547, V_{p² σ} → -1.1006}],
{kx, -3.3, 0}, {ky, 0, 2.}, PlotLegends → Automatic, AspectRatio → Equal]
```
wykres gęstości; wartość bezwzględna; legenda dla grafik; automatyczny; format obrazu; równe

Out[57]=



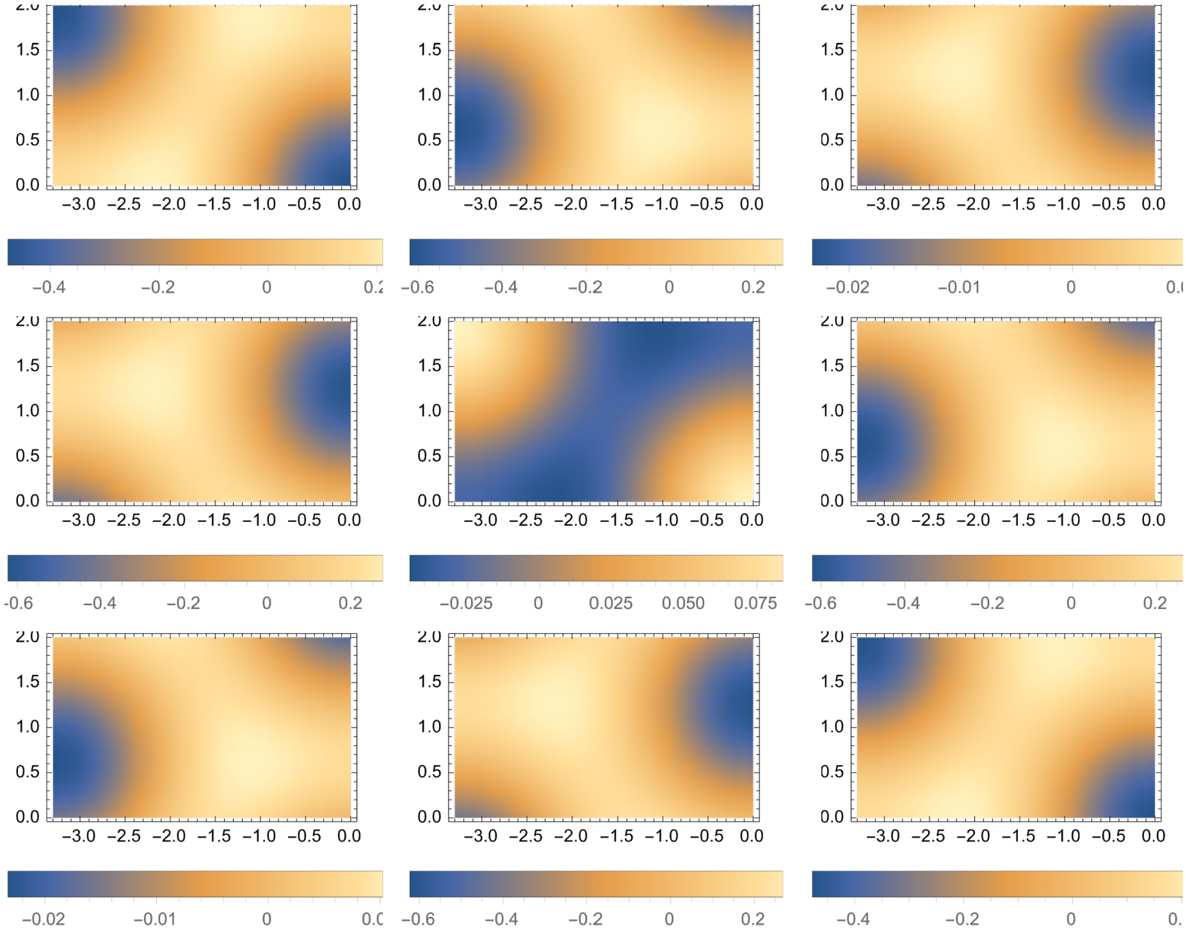
```
In[83]:= HoppingKRe[i_, j_] := DensityPlot[
                                 wykres gęstości
    Re[HSKinter[[i, j]] /. {dr → 3.323 / √3 , dzpp → 3.05, dzdd → 6.4, Vd²π → 1.8318,
    część rzeczywista
        Vd²δ → -0.3299, Vd²σ → -0.5, Vp²π → -0.1547, Vp²σ → -1.1006}], {kx, -3.3, 0},
    {ky, 0, 2.}, PlotLegends → Placed[Automatic, Below], AspectRatio → Equal];
                 legenda dla grafik  umieść  automatyczny  poniżej  format obrazu  równe

HoppingKIm[i_, j_] := DensityPlot[
                      wykres gęstości
    Im[HSKinter[[i, j]] /. {dr → 3.323 / √3 , dzpp → 3.05, dzdd → 6.4, Vd²π → 1.8318,
    część urojona
        Vd²δ → -0.3299, Vd²σ → -0.5, Vp²π → -0.1547, Vp²σ → -1.1006}], {kx, -3.3, 0},
    {ky, 0, 2.}, PlotLegends → Placed[Automatic, Below], AspectRatio → Equal];
                 legenda dla grafik  umieść  automatyczny  poniżej  format obrazu  równe

DDRe = Table[HoppingKRe[i, j], {i, 1, 3}, {j, 1, 3}];
       tabela
DDIm = Table[HoppingKIm[i, j], {i, 1, 3}, {j, 1, 3}];
       tabela
PPRe = Table[HoppingKRe[i, j], {i, 4, 6}, {j, 4, 6}];
       tabela
PPIm = Table[HoppingKIm[i, j], {i, 4, 6}, {j, 4, 6}];
       tabela
```

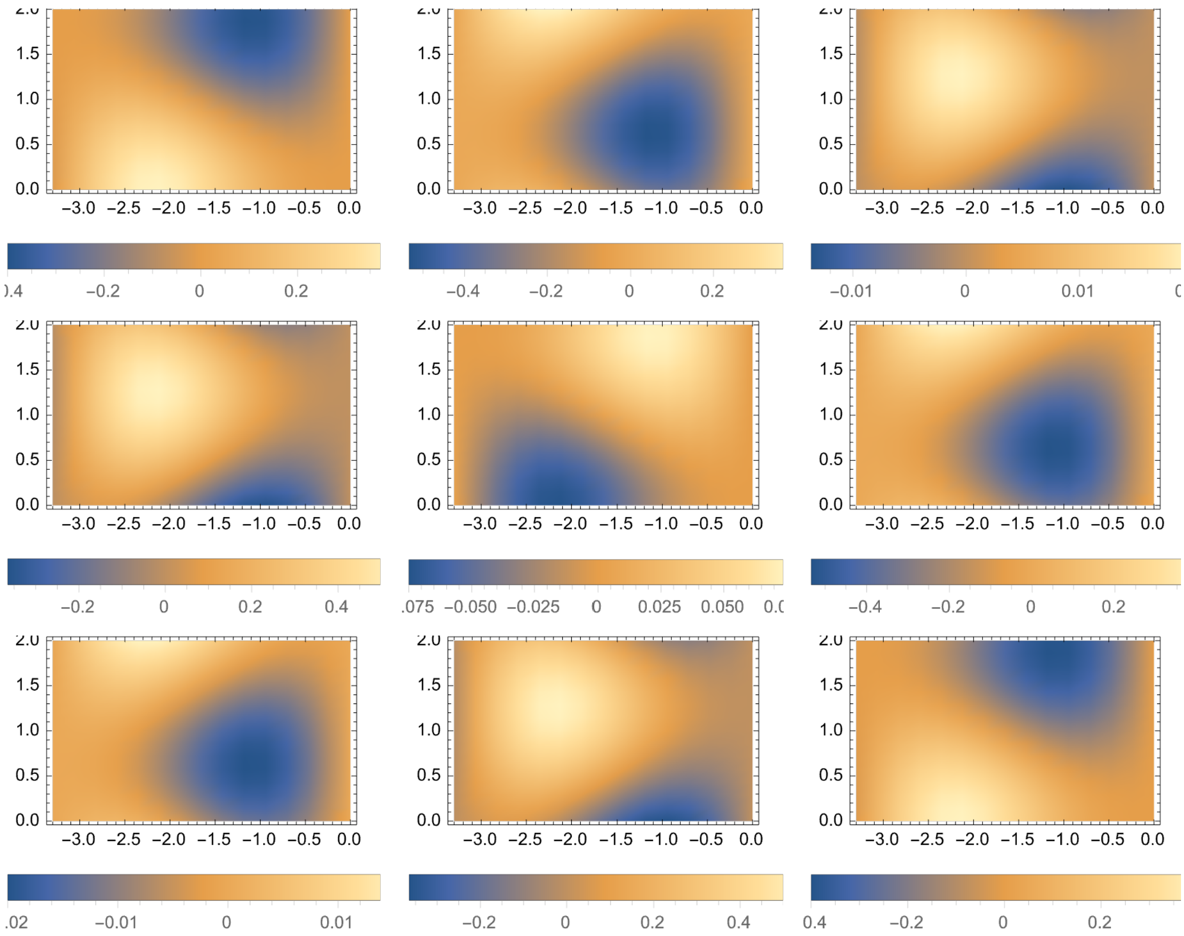
In[89]:= `GraphicsGrid[DDRe]`
siatka z grafikami

Out[89]=



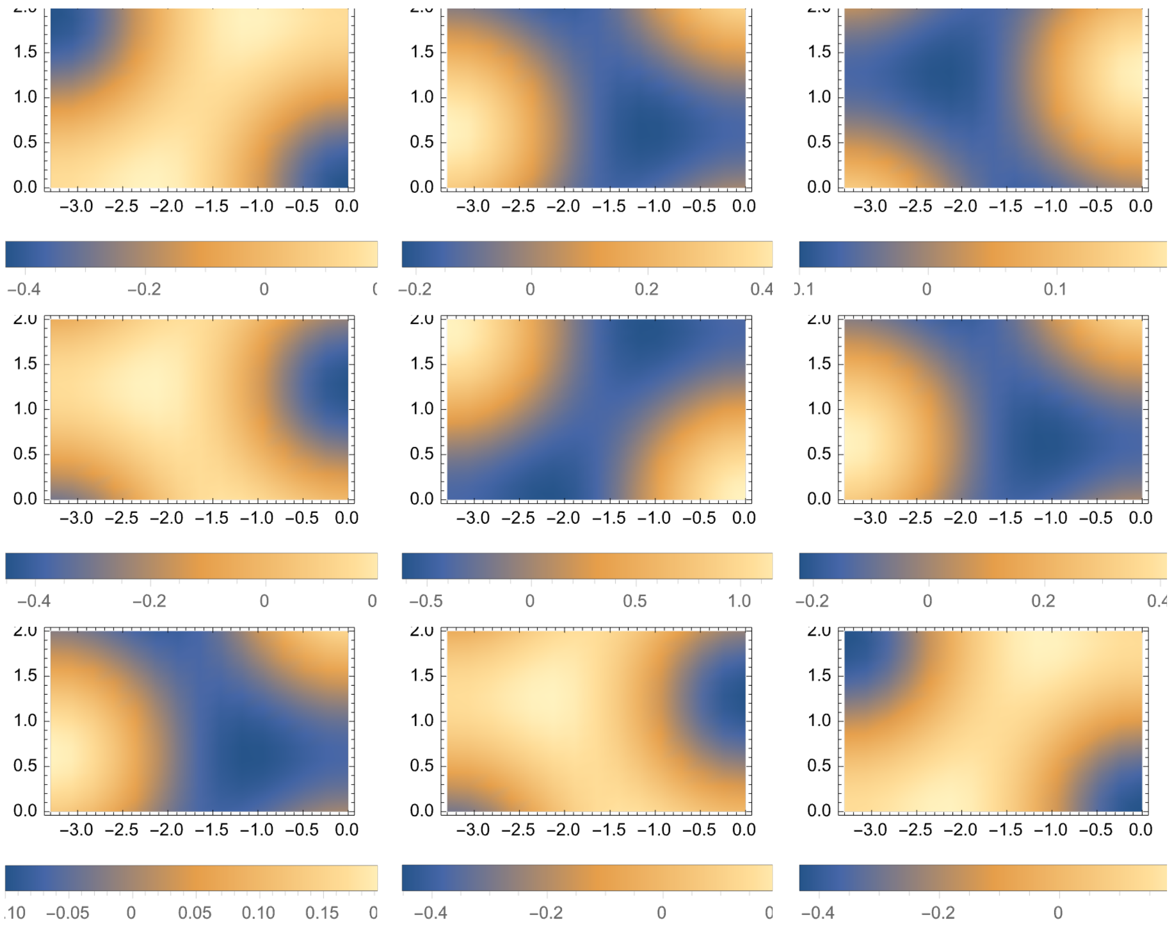
In[90]:=
```
GraphicsGrid[DDIm]
```
siatka z grafikami

Out[90]=



In[91]:=
```
GraphicsGrid[PPRe]
```
siatka z grafikami

Out[91]=



In[92]:= `GraphicsGrid[PPIm]`

siatka z grafikami

Out[92]=