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

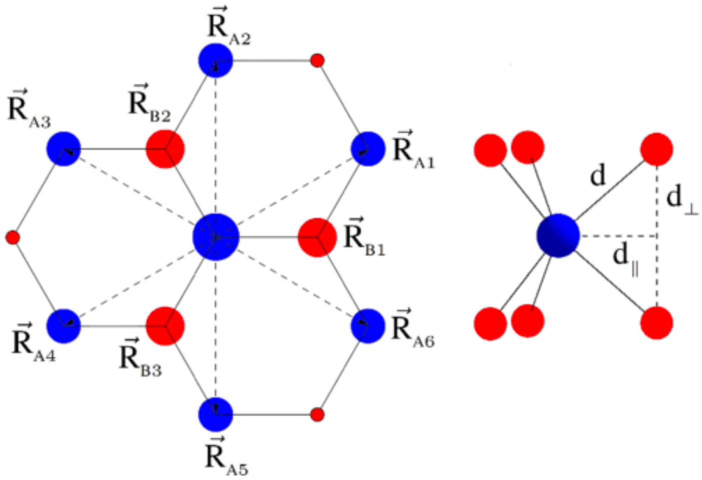
TMDC monolayer : 3-band model

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

In[6]:=



;

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[7]:= Dp2 = 1/Sqrt[2] (x2y2 + I xy);(*even orbital at M*)
                          ⌊jedność urojona

Dp1 = -1/Sqrt[2] (xz + I yz);(*odd orbital at M*)
                        ⌊jedność urojona

D0 = z2;(*even orbital at M*)
Dm1 = 1/Sqrt[2] (xz - I yz);(*odd orbital at M*)
                        ⌊jedność urojona

Dm2 = 1/Sqrt[2] (x2y2 - I xy);(*even orbital at M*)
                          ⌊jedność urojona

PEp1 = {-1/2 (x + I y), -1/2 (x + I y)};
              ⌊jedność urojona  ⌊jedność urojona

(*even X2 dimer composed of up and down orbital*)
PE0 = {1/Sqrt[2] z, -1/Sqrt[2] z}; (*even X2 dimer composed of up and down orbital*)
PEm1 = {1/2 (x - I y), 1/2 (x - I y)};
             ⌊jedność urojona ⌊jedność urojona

(*even X2 dimer composed of up and down orbital*)
POp1 = {-1/2 (x + I y), 1/2 (x + I y)};
              ⌊jedność urojona ⌊jedność urojona

(*odd X2 dimer composed of up and down orbital*)
PO0 = {1/Sqrt[2] z, 1/Sqrt[2] z};(*odd X2 dimer composed of up and down orbital*)
POm1 = {1/2 (x - I y), 1/2 (-x + I y)};
             ⌊jedność urojona  ⌊jedność urojona

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

Collect all basis elements :

```
In[18]:= 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)

In[19]:=
$$\text{hopMM} = \left\{\left\{\frac{3}{2}\,\text{dr},\ \frac{\sqrt{3}}{2}\,\text{dr},\ 0\right\},\ \left\{0,\ \sqrt{3}\,\text{dr},\ 0\right\},\ \left\{-\frac{3}{2}\,\text{dr},\ \frac{\sqrt{3}}{2}\,\text{dr},\ 0\right\},\ \left\{-\frac{3}{2}\,\text{dr},\ -\frac{\sqrt{3}}{2}\,\text{dr},\ 0\right\},\ \left\{0,\ -\sqrt{3}\,\text{dr},\ 0\right\},\ \left\{\frac{3}{2}\,\text{dr},\ -\frac{\sqrt{3}}{2}\,\text{dr},\ 0\right\}\right\};$$

$$\text{mxu} = \left\{\{\text{dr},\ 0,\ \text{dp}\},\ \left\{-\frac{1}{2}\,\text{dr},\ \frac{\sqrt{3}}{2}\,\text{dr},\ \text{dp}\right\},\ \left\{-\frac{1}{2}\,\text{dr},\ -\frac{\sqrt{3}}{2}\,\text{dr},\ \text{dp}\right\}\right\};$$

$$\text{xum} = \left\{\{-\text{dr},\ 0,\ -\text{dp}\},\ \left\{\frac{1}{2}\,\text{dr},\ -\frac{\sqrt{3}}{2}\,\text{dr},\ -\text{dp}\right\},\ \left\{\frac{1}{2}\,\text{dr},\ \frac{\sqrt{3}}{2}\,\text{dr},\ -\text{dp}\right\}\right\};$$

$$\text{mxd} = \left\{\{\text{dr},\ 0,\ -\text{dp}\},\ \left\{-\frac{1}{2}\,\text{dr},\ \frac{\sqrt{3}}{2}\,\text{dr},\ -\text{dp}\right\},\ \left\{-\frac{1}{2}\,\text{dr},\ -\frac{\sqrt{3}}{2}\,\text{dr},\ -\text{dp}\right\}\right\};$$

$$\text{xdm} = \left\{\{-\text{dr},\ 0,\ \text{dp}\},\ \left\{\frac{1}{2}\,\text{dr},\ -\frac{\sqrt{3}}{2}\,\text{dr},\ \text{dp}\right\},\ \left\{\frac{1}{2}\,\text{dr},\ \frac{\sqrt{3}}{2}\,\text{dr},\ \text{dp}\right\}\right\};$$

```
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[27]:=
```
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[28]:=
```
GetHoppingSingle[D0, D0, x, y, z]
```

Out[28]=

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

In[29]:=
```
FullSimplify[GetHopping[Dm1, P0p1,
  {{{dr, 0, dp}}, {{dr, 0, -dp}}, {1, 2}}, True] /. {dp^2 + dr^2 → d^2}]
```
uprość pełniej, prawda

Out[29]=

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

In[30]:=
```
FullSimplify[GetHopping[Dm2, D0, {{3/2 dr, √3/2 dr, 0}}, True]]
```
uprość pełniej, prawda

Out[30]=

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

Matrix elements

In[31]:=
```
H1v1 = FullSimplify[GetHopping[D0, D0, hopMM, True]]
```
uprość pełniej, prawda

Out[31]=

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

In[32]:=
```
FullSimplify[
  H1v1 == 1/2 (3 V_{d² δ} + V_{d² σ}) (2 Cos[3 / 2 kx dr] * Cos[√3 / 2 ky dr] + Cos[√3 ky dr])]
```
uprość pełniej, cosinus, cosinus, cosinus

Out[32]=
```
True
```

In[33]:=

```
H1v2 = FullSimplify[GetHopping[Dm2, D0, hopMM, True]]
```

uprość pełniej prawda

Out[33]=

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

In[34]:=

$$\text{FullSimplify}\left[\text{H1v2}==\frac{-\sqrt{3}}{2\sqrt{2}}\left(V_{d^2\,\sigma}-V_{d^2\,\delta}\right)\left(\text{Cos}\left[3/2\,\text{kx dr}+\sqrt{3}\,/\,2\,\text{ky dr}\right]\text{Exp[I Pi / 3]}+\text{Cos}\left[3/2\,\text{kx dr}-\sqrt{3}\,/\,2\,\text{ky dr}\right]\text{Exp[-I Pi / 3]}-\text{Cos}\left[\sqrt{3}\,\text{ky dr}\right]\right)\right]$$

uprość pełniej cosinus fu⋯ ⋅ pi cosinus funkc⋯ ⋅ pi cosinus

Out[34]=

True

In[35]:=

```
H5v5 = FullSimplify[GetHopping[PE0, PE0, hopXX, True]]
```

uprość pełniej prawda

Out[35]=

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

In[36]:=

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

uprość pełniej cosinus cosinus cosinus

Out[36]=

True

In[37]:=

```
H4v6 = FullSimplify[GetHopping[PEm1, PEp1, hopXX, True]]
```

uprość pełniej prawda

Out[37]=

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

In[38]:=

$$\text{FullSimplify}\left[\text{H4v6}==\left(V_{p^2\,\sigma}-V_{p^2\,\pi}\right)\left(\text{Cos}\left[3/2\,\text{kx dr}+\sqrt{3}\,/\,2\,\text{ky dr}\right]\text{Exp[I Pi / 3]}+\text{Cos}\left[3/2\,\text{kx dr}-\sqrt{3}\,/\,2\,\text{ky dr}\right]\text{Exp[-I Pi / 3]}-\text{Cos}\left[\sqrt{3}\,\text{ky dr}\right]\right)*(-1)\right]$$

uprość pełniej cosinus fu⋯ ⋅ pi cosinus funkc⋯ ⋅ pi cosinus

Out[38]=

True

In[39]:=

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

uprość pełniej prawda

Out[39]=

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

In[40]:=

$$\text{FullSimplify}\Big[\text{H3v6} == \frac{dr}{\sqrt{2}\ d}\left(\sqrt{3}\Big/2\ V_{dp\sigma}\left(dp^2/d^2-1\right)-V_{dp\pi}\left(dp^2/d^2+1\right)\right)$$

$$\left(\text{Exp}[\text{I kx dr}]+\text{Exp}\left[-\text{I kx dr}/2+\text{I}\sqrt{3}\ \text{ky dr}/2-2\ \text{I Pi}/3\right]+\text{Exp}\left[-\text{I kx dr}/2-\text{I}\sqrt{3}\ \text{ky dr}/2+2\ \text{I Pi}/3\right]\right)*(-1),$$

$$\{d\in\text{Reals},\ d>0\}\Big]\ /.\ \left\{dp^2+dr^2\to d^2\right\}$$

uprość pełniej; fu⋯ jedność ur⋯ funkc⋯ jedność urojona jedność urojona ⋅ pi; funkc⋯ jedność urojona jedność urojona ⋅ pi; liczby rzeczywiste

Out[40]=

True

In[41]:=

```
H7v11 = FullSimplify[GetHopping[Dm1, POp1, hopMX, True] /. {dp² + dr² → d²}]
```

uprość pełniej; prawda

Out[41]=

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

In[42]:=

$$\text{FullSimplify}\Big[\text{H7v11} == -\frac{dp\ dr^2}{\sqrt{2}\ d^3}\left(\sqrt{3}\ V_{dp\sigma}-2\ V_{dp\pi}\right)$$

$$\left(\text{Exp}[\text{I kx dr}]+\text{Exp}\left[-\text{I kx dr}/2+\text{I}\sqrt{3}\ \text{ky dr}/2-2\ \text{I Pi}/3\right]+\text{Exp}\left[-\text{I kx dr}/2-\text{I}\sqrt{3}\ \text{ky dr}/2+2\ \text{I Pi}/3\right]\right)*(-1),$$

$$\{d\in\text{Reals},\ d>0\}\Big]\ /.\ \left\{dp^2+dr^2\to d^2\right\}$$

uprość pełniej; fu⋯ jedność ur⋯ funkc⋯ jedność urojona jedność urojona ⋅ pi; funkc⋯ jedność urojona jedność urojona ⋅ pi; liczby rzeczywiste

Out[42]=

True

In[43]:=

```
H7v10 = FullSimplify[GetHopping[Dm1, PO0, hopMX, True] /. {dp² + dr² → d²}]
```

uprość pełniej; prawda

Out[43]=

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

In[44]:=

```
FullSimplify[H7v10 == -(dr/d) ((dp^2/d^2) (Sqrt[3] Vdpσ - 2 Vdpπ) + 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]), {d ∈ Reals, d > 0}] /. {dp^2 + dr^2 → d^2}
```

uprość pełniej; fu··· jedność ur··· funkc··· jedność urojona jedność urojona ·· pi funkcja eksponencjalna; jedność urojona jedność urojona ·· pi liczby rzeczywiste

Out[44]=

True

In[45]:=

```
H8v9 = FullSimplify[GetHopping[Dp1, POm1, hopMX, True] /. {dp^2 + dr^2 → d^2}]
```

uprość pełniej; prawda

Out[45]=

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

In[46]:=

```
FullSimplify[H8v9 ==
   (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]),
  {d ∈ Reals, d > 0}] /. {dp^2 + dr^2 → d^2}
```

uprość pełniej; fu··· jedność ur··· funkc··· jedność urojona jedność urojona ·· pi; funkc··· jedność urojona jedność urojona ·· pi; liczby rzeczywiste

Out[46]=

True

In[47]:=

```
H8v10 = FullSimplify[GetHopping[Dp1, PO0, hopMX, True] /. {dp^2 + dr^2 → d^2}]
```

uprość pełniej; prawda

Out[47]=

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

In[48]:=
```
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]), {d ∈ Reals, d > 0}] /. {dp^2 + dr^2 → d^2}
```
uprość pełniej; fu⋯; jedność ur⋯; funkc⋯; jedność urojona; jedność urojona; pi; funkcja eksponencjalna; jedność urojona; jedność urojona; pi; liczby rzeczywiste

Out[48]=
True

In[49]:=
```
H9v11 = FullSimplify[GetHopping[POm1, POp1, hopXX, True] /. {dp^2 + dr^2 → d^2}]
```
uprość pełniej; prawda

Out[49]=

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

In[50]:=
```
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)]
```
uprość pełniej; cosinus; fu⋯; pi; cosinus; funkc⋯; pi; cosinus

Out[50]=
True

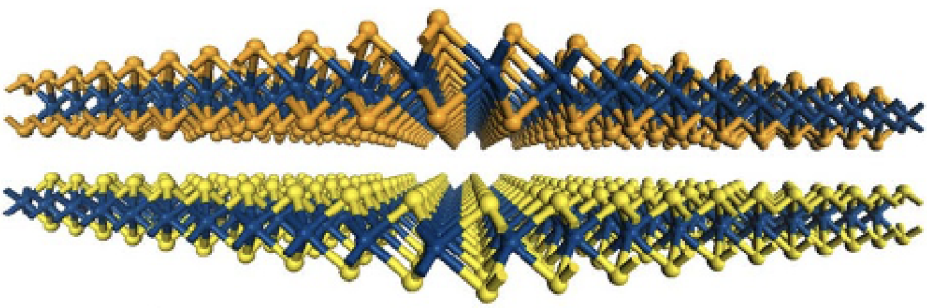
In[51]:=
```
H9v10 = FullSimplify[GetHopping[POm1, PO0, hopXX, True] /. {dp^2 + dr^2 → d^2}]
```
uprość pełniej; prawda

Out[51]=
0

TMDC heterostructure

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

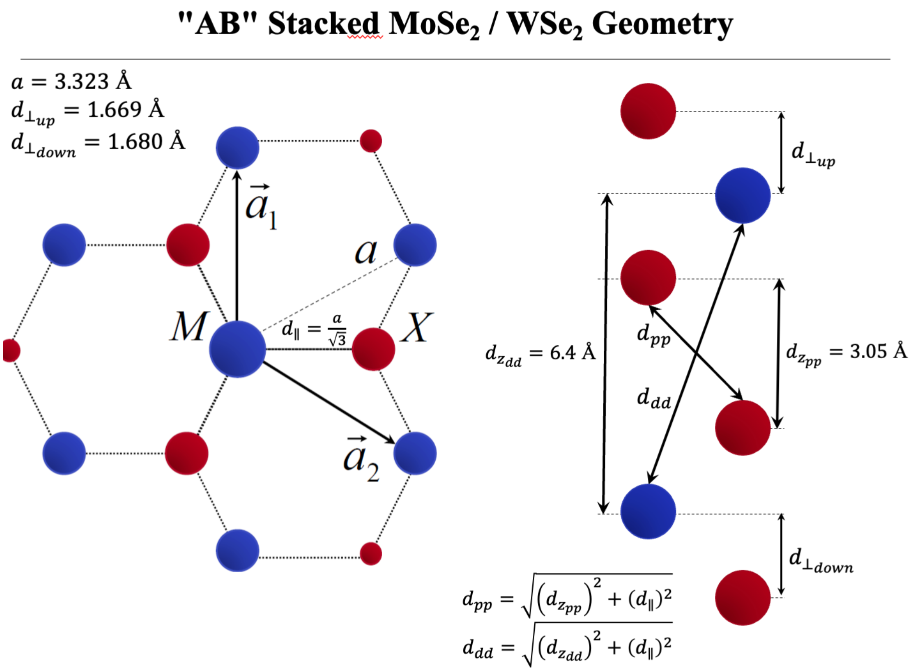
In[52]:=



;

Interalyer hoppings

In[53]:=



;

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

In[54]:=

$$\texttt{ihopMM = List}\left[\{-\texttt{dr}, 0, -\texttt{dzdd}\}, \left\{\frac{1}{2}\,\texttt{dr}, -\frac{\sqrt{3}}{2}\,\texttt{dr}, -\texttt{dzdd}\right\}, \left\{\frac{1}{2}\,\texttt{dr}, \frac{\sqrt{3}}{2}\,\texttt{dr}, -\texttt{dzdd}\right\}\right];$$

lista

```
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 *)
```

$$\texttt{ihopxx = List}\left[\{\texttt{dr}, 0, -\texttt{dzpp}\}, \left\{-\frac{1}{2}\,\texttt{dr}, \frac{\sqrt{3}}{2}\,\texttt{dr}, -\texttt{dzpp}\right\}, \left\{-\frac{1}{2}\,\texttt{dr}, -\frac{\sqrt{3}}{2}\,\texttt{dr}, -\texttt{dzpp}\right\}\right];$$

lista

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

In[59]:=

```
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[60]:=

```
Iorbitals = {Dm2, D0, Dp2, PEm1, PE0, PEp1};
```

In[61]:=
```
HSKinter = HSKHoppings[Iorbitals, IHop, True];
(* last parameter means that we want to print elements out *)
```
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]

$$\frac{\text{dzdp}\ V_{\text{dp}\sigma}}{\sqrt{2}\ \sqrt{\text{dzdp}^2}}$$

[2,6]

0

[3,1]

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

[3,2]

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

[3,3]

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

[3,4]

0

[3,5]

0

[3,6]

0

[4,1]

0

[4,2]

0

[4,3]

0

[4,4]

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

[4,5]

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

[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]

$$\frac{dzdp\; V_{pd\sigma}}{\sqrt{2}\,\sqrt{dzdp^2}}$$

[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]

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

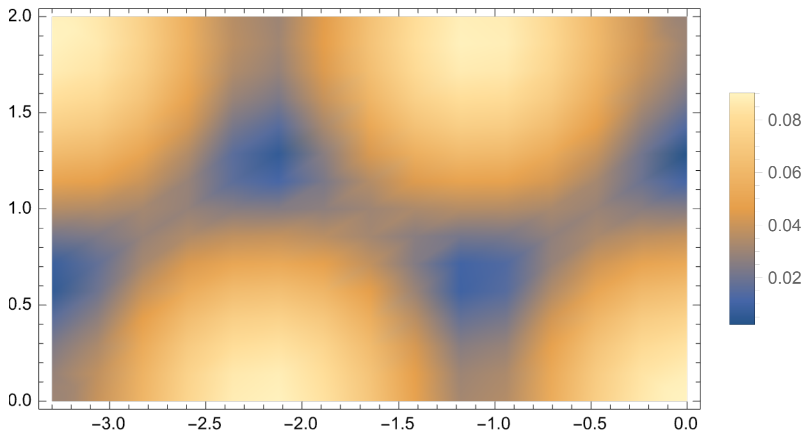
Now save the whole intelayer block in *.f file (to be parsed in python)

```
In[62]:= IHop = {
    {ihopMM, ihopMM, ihopMM, ihopMX,
     ihopMX, ihopMX, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopMM, ihopMM, ihopMM, ihopMX,
     ihopMX, ihopMX, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopMM, ihopMM, ihopMM, ihopMX,
     ihopMX, ihopMX, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopXM, ihopXM, ihopXM, ihopXX,
     ihopXX, ihopXX, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX},
    {ihopXM, ihopXM, ihopXM, ihopXX,
     ihopXX, ihopXX, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX},
    {ihopXM, ihopXM, ihopXM, ihopXX,
     ihopXX, ihopXX, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX},
    {ihopMM, ihopMM, ihopMM, ihopMX,
     ihopMX, ihopMX, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopMM, ihopMM, ihopMM, ihopMX,
     ihopMX, ihopMX, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopXM, ihopXM, ihopXM, ihopXX,
     ihopXX, ihopXX, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX},
    {ihopXM, ihopXM, ihopXM, ihopXX,
     ihopXX, ihopXX, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX},
    {ihopXM, ihopXM, ihopXM, ihopXX,
     ihopXX, ihopXX, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX}
   };

In[63]:= Iorbitals = {Dm2, D0, Dp2, PEm1, PE0, PEp1, Dm1, Dp1, POm1, PO0, POp1};

In[64]:= HSKinter = HSKHoppings[Iorbitals, IHop, False];
                                                      fałsz

In[65]:= SetDirectory[NotebookDirectory[]];
         ustaw katalog ro··· katalog notatnika
         stream = OpenWrite["interlayer.f"];
                  otwórz do zapisu
         For[i = 1, i ≤ 11, i++,
         dla
          For[j = 1, j ≤ 11, j++,
          dla
           str = StringForm["H_k[`1`,`2`]=`3`", i, 11 + j, FortranForm[HSKinter[[i, j]]]];
                 forma ciągu znaków                        zapisz w Fortran
           WriteString[stream, ToString[str, OutputForm]];
           napisz ciąg         przemień na ciąg ···  formularz wyjścia
           WriteString[stream, "\n"]
           napisz ciąg
          ]
         ]
         Close[stream];
         zamknij strumień
```

Elements analysis

In[69]:=
```
DensityPlot[
wykres gęstości
 Abs[HSKinter[[2, 2]] /. {dr → 3.323 / √3, dzpp → 3.05, dzdd → 6.4, V_{d² π} → 1.8318,
 wartość bezwzględna
    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]
                              legenda dla grafik  automatyczny  format obrazu  równe
```

Out[69]=



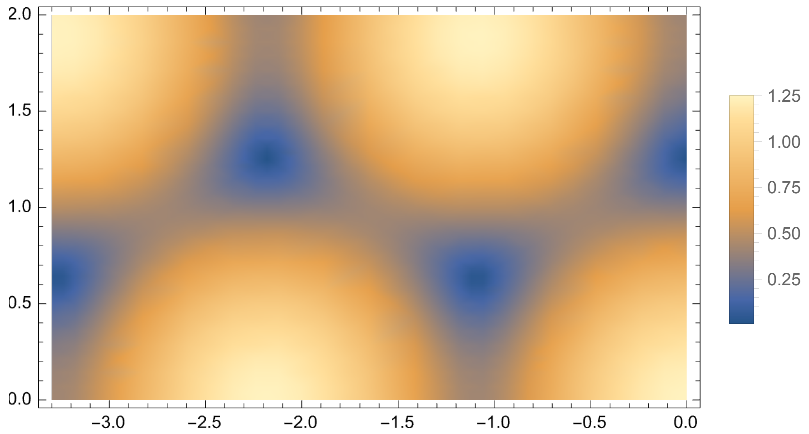
In[70]:=
```
HSKinter[[5, 5]] (*P0-P0*)
```

Out[70]=

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

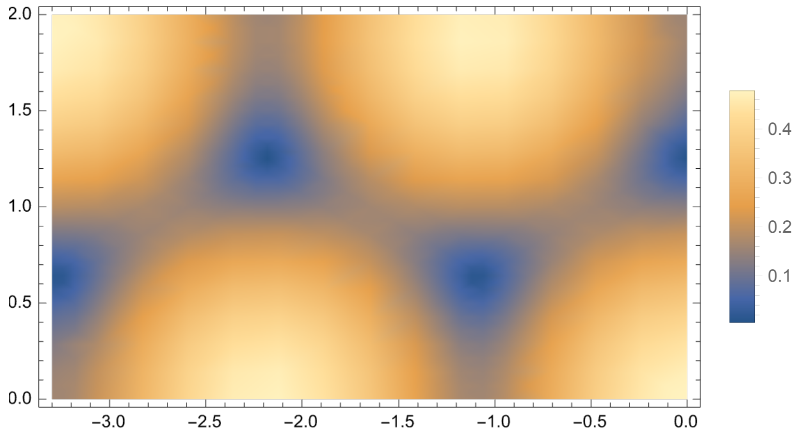
In[71]:=
```
DensityPlot[
wykres gęstości
  Abs[HSKinter[[5, 5]] /. {dr → 3.323/ √3 , dzpp → 3.05, dzdd → 6.4, V_{d² π} → 1.8318,
  wartość bezwzględna
     V_{d² δ} → -0.3299, V_{d² σ} → -0.5, V_{p² π} → -0.1547, V_{p² σ} → -1.1006}],
  {kx, -3.3, 0}, {ky, 0, 2.0}, PlotLegends → Automatic, AspectRatio → Equal]
                               legenda dla grafik    automatyczny  format obrazu    równe
```

Out[71]=



In[72]:=
```
DensityPlot[
wykres gęstości
  Abs[HSKinter[[1, 1]] /. {dr → 3.323/ √3 , dzpp → 3.05, dzdd → 6.4, V_{d² π} → 1.8318,
  wartość bezwzględna
     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]
                             legenda dla grafik    automatyczny  format obrazu    równe
```

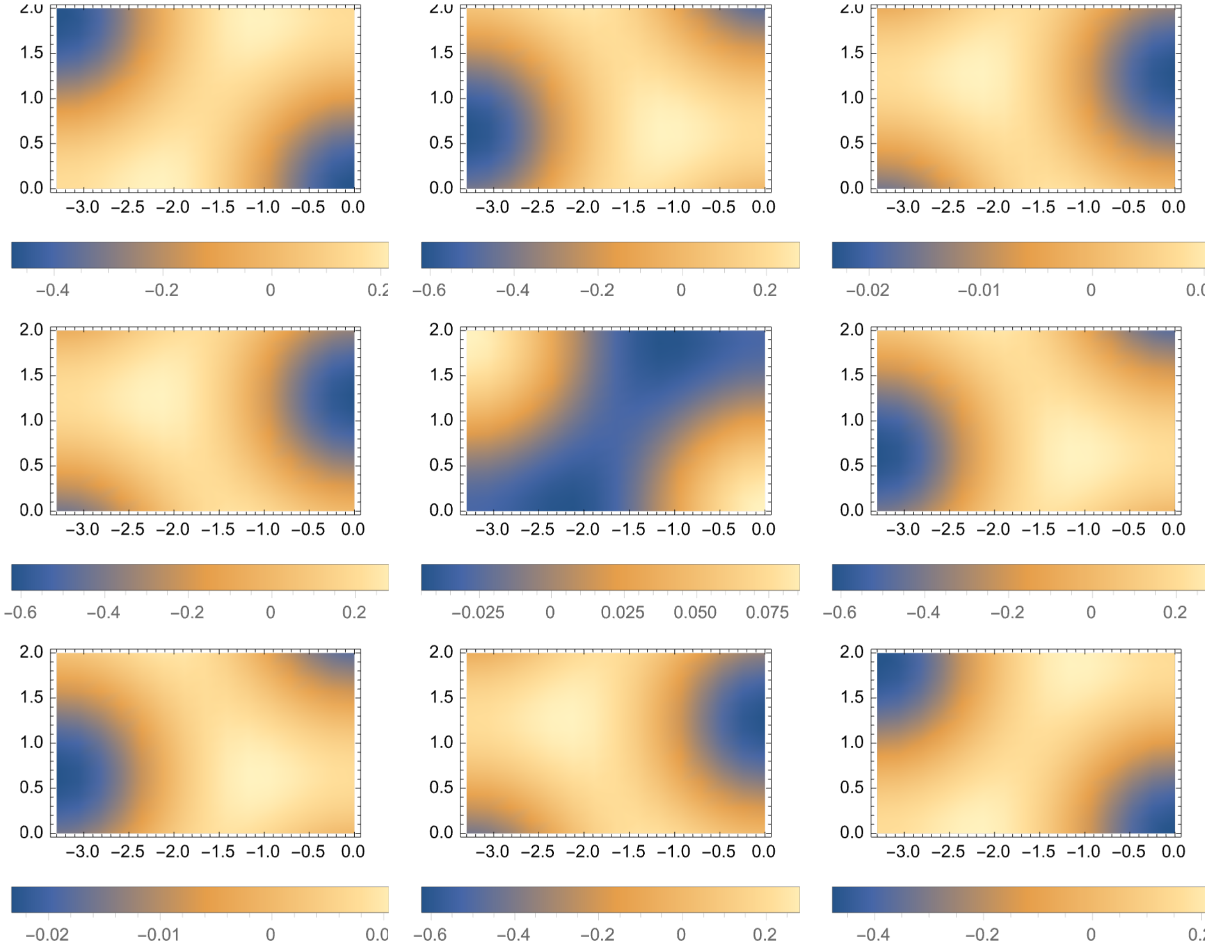
Out[72]=



In[73]:=
```
HoppingKRe[i_, j_] := DensityPlot[
                      wykres gęstości
  Re[HSKinter[[i, j]] /. {dr → 3.323/√3, dzpp → 3.05, dzdd → 6.4, V_{d² π} → 1.8318,
  część rzeczywista
     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 → 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, V_{d² π} → 1.8318,
  część urojona
     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 → 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
```

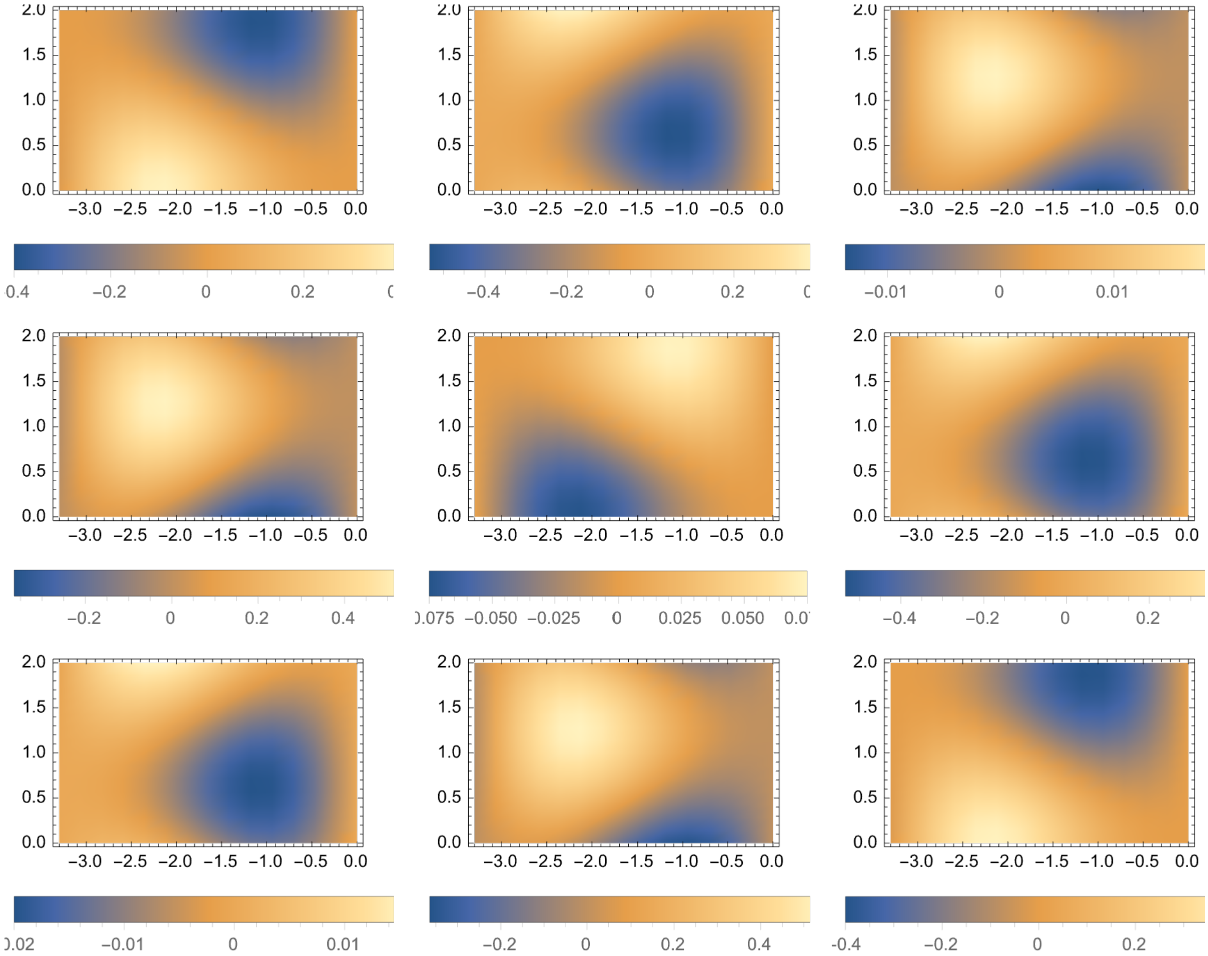
In[79]:=
```
GraphicsGrid[DDRe]
```
siatka z grafikami

Out[79]=



In[80]:=
```
GraphicsGrid[DDIm]
```
siatka z grafikami

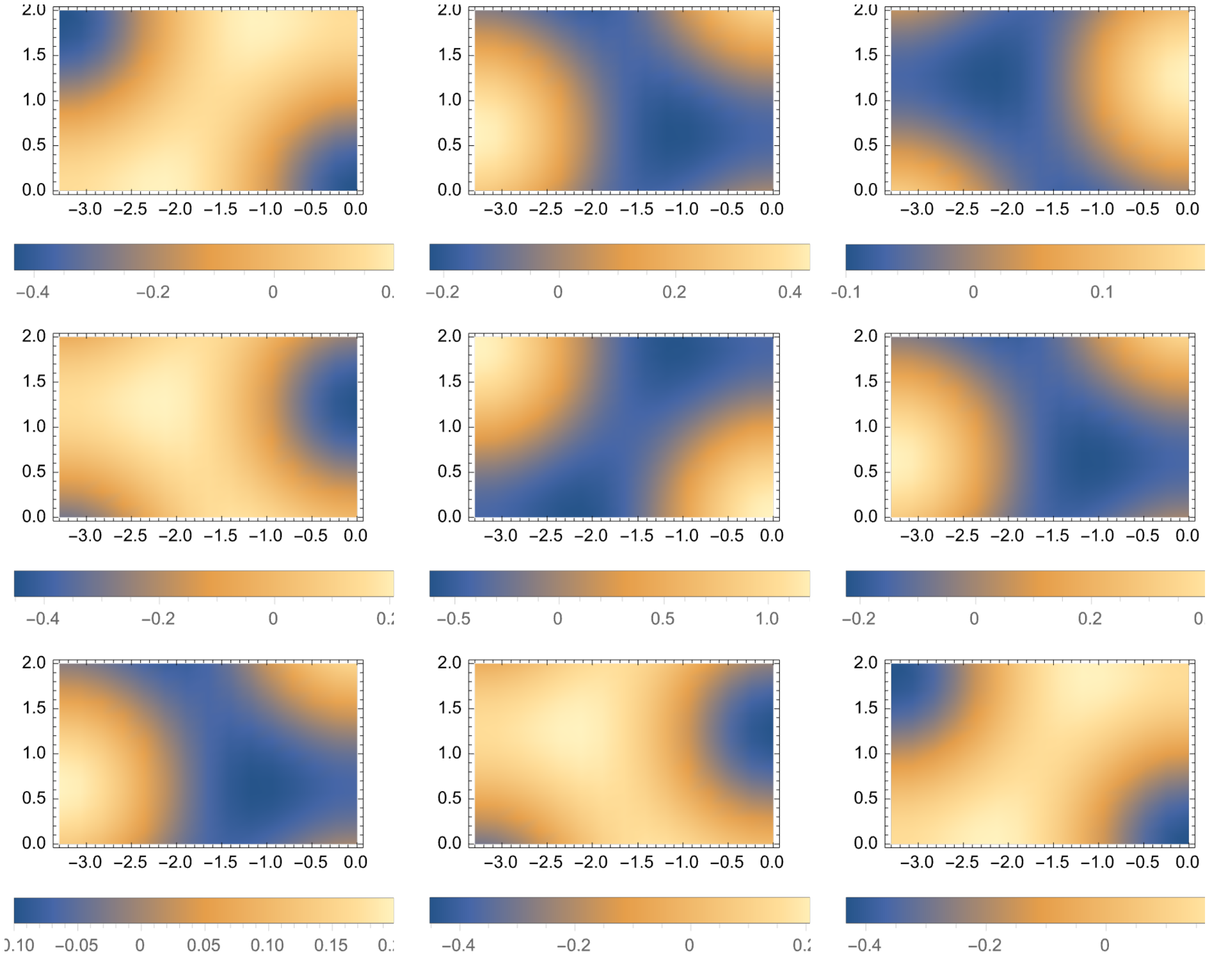
Out[80]=



In[81]:= `GraphicsGrid[PPRe]`

siatka z grafikami

Out[81]=



In[82]:=
```
GraphicsGrid[PPIm]
```
siatka z grafikami

Out[82]=