In[1]:=
```
Needs["Quanty`TightBinding`"]
Needs["Quanty`PlotTools`"]
```

```
Loaded Quanty : Tight Binding package - version 2016.1.27

Written by Maurits W. Haverkort

Loaded the Quanty : Plot Tools Package - version 2016.1.27

Written by Maurits W. Haverkort
```

Topological surface state

In these notes we create a simple tight binding model that shows a topological non-trivial system. We then create a slab using this model and discuss the surface states that “have to” rise between a topological trivial (vacuum) and non-trivial (by construction) state.

Bulk

The model we use is a tight binding model of a square lattice.
On each site there is a s and a p orbital.
The tight binding Hamiltonian is thus a 4 by 4 matrix and has the parameters: ϵs,ϵp,ssσ,spσ, and ppσ.
We will later add spin-orbit coupling and thus the spin-orbit coupling constant (ζ) is a parameter as well.

In[3]:=
```
ClearAll[εs, εp, ssσ, spσ, ppσ, ζ]
```

The basis of our Hamiltonian is px, py, pz and the s orbital. Only nearest neighbor hopping of σ type is included

In[4]:=
```
H = ⎛ εp + ppσ (e^(i π κx) + e^(-i π κx))   0                                   0                                   spσ (e^(i π κx) - e^(-i π κx))   ⎞
    ⎜ 0                                     εp + ppσ (e^(i π κy) + e^(-i π κy)) 0                                   spσ (e^(i π κy) - e^(-i π κy))   ⎟
    ⎜ 0                                     0                                   εp + ppσ (e^(i π κz) + e^(-i π κz)) spσ (e^(i π κz) - e^(-i π κz))   ⎟
    ⎝ spσ (-e^(i π κx) + e^(-i π κx))       spσ (-e^(i π κy) + e^(-i π κy))     spσ (-e^(i π κz) + e^(-i π κz))     εs + ssσ (e^(i π κx) + e^(-i π κx) + e^(i π κy) + e^(-i π κy) + e^(i π κz) + e^(-i π κz)) ⎠ ;
```

To plot a band structure, the path in k-space is given as:

In[5]:=
```
KPathDefine = {
    {"R", {1, 1, 1}, 87},
    {"Γ", {0, 0, 0}, 50},
    {"X", {1, 0, 0}, 50},
    {"M", {1, 1, 0}, 71},
    {"Γ", {0 , 0,  0}, 1},
    {"Γ", {0 , 0 , 0}, 0}
   };
```

Let's define colors for the bands: s band will be blue, the p bands in red. Here, we first do it for NO spin-orbit coupling

In[6]:=
```
CharacterToColor[Character_] := Module[{VRed, VGreen, VBlue},
  VRed = Character[[{1, 2, 3}]].Character[[{1, 2, 3}]]*;
  VGreen = 0;
  VBlue = Character[[{4}]].Character[[{4}]]*;
  RGBColor[VRed, VGreen, VBlue]]
```

The same needs to be done for the calculation with spin-orbit coupling. In this case a slightly different function is needed as the basis size is different (both spin up and down are in the basis)

In[7]:=
```
CharacterToColorSOC[Character_] := Module[{VRed, VGreen, VBlue},
  VRed = Character[[{1, 2, 3, 5, 6, 7}]].Character[[{1, 2, 3, 5, 6, 7}]]*;
  VGreen = 0;
  VBlue = Character[[{4, 8}]].Character[[{4, 8}]]*;
  RGBColor[VRed, VGreen, VBlue]]
```

We can define a function for the line thickness

In[8]:=
```
CharacterToThickness[Character_] := Module[{},
  Thickness[0.005 + 0.01 Character[[{4}]].Character[[{4}]]*]
 ]
```

And again a slightly different function for the case with spin-orbit coupling

In[9]:=
```
CharacterToThicknessSOC[Character_] := Module[{},
  Thickness[0.005 + 0.01 Character[[{4, 8}]].Character[[{4, 8}]]*]
 ]
```

The list of k-points is generated

In[10]:=
```
KPoints = Flatten[Table[
    Table[KPathDefine[[i, 2]] (KPathDefine[[i, 3]] - j + 1) / KPathDefine[[i, 3]] +
      KPathDefine[[i + 1, 2]] (j - 1) / KPathDefine[[i, 3]],
     {j, 1, KPathDefine[[i, 3]]}], {i, 1, Length[KPathDefine] - 1}], 1];
```

and a list of names belonging to some k points

In[11]:=
```
Knames = Table[{KPathDefine[[i, 1]], 1 + Sum[KPathDefine[[ii, 3]], {ii, 1, i - 1}]},
   {i, 1, Length[KPathDefine] - 1}];
```

In[12]:=

As a first start, we set the parameters such that the Hamiltonian does not include p and s mixing terms.

In[13]:=
```
ϵp = 4.1;
ϵs = 9;
ssσ = -3;
ppσ = 2;
spσ = 0;
HNointeractionfun[κx_, κy_, κz_] := Evaluate[N[H]];
```

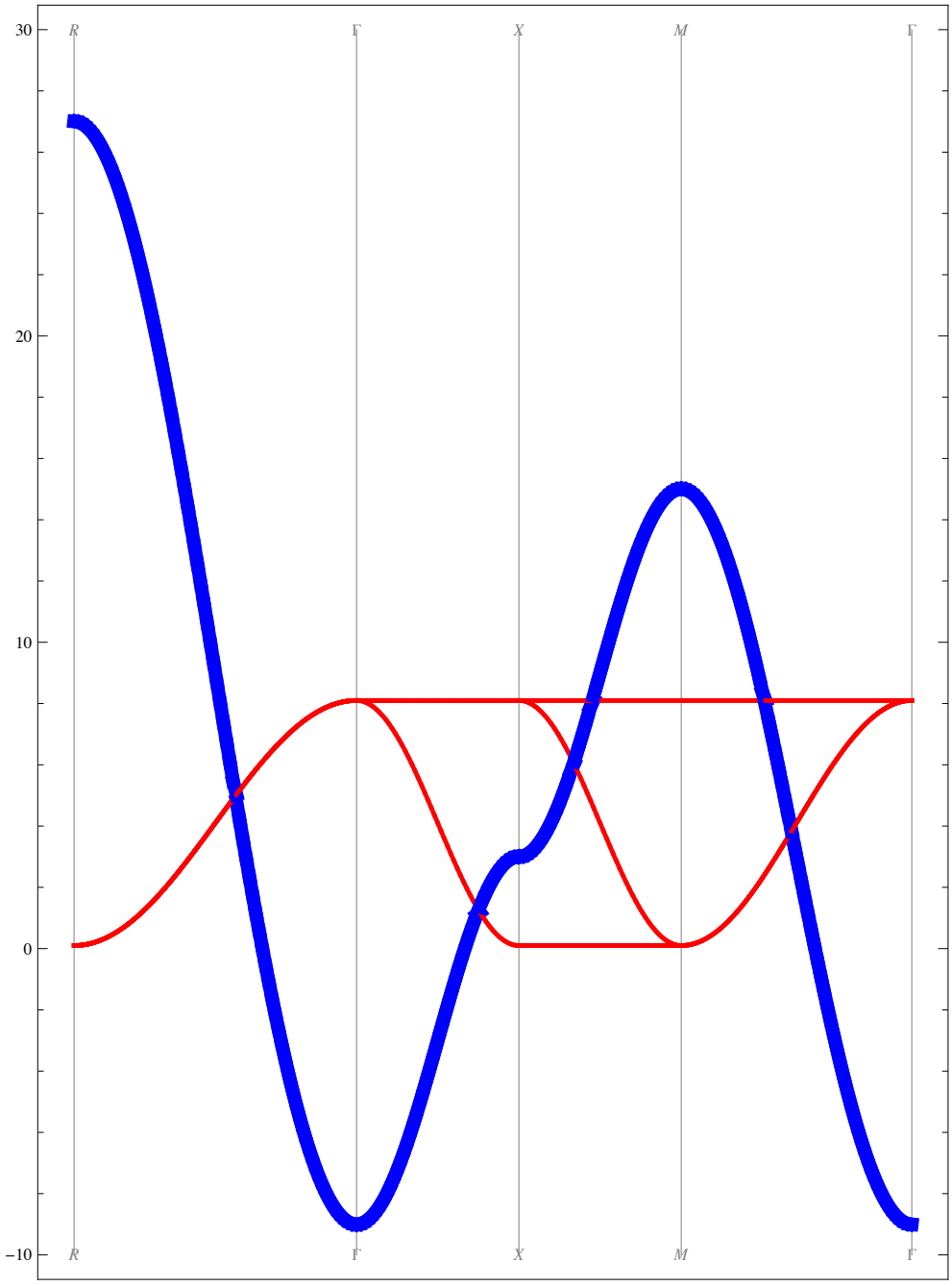
We can calculate the eigen-states at the k-points defined above

In[19]:=
```
{TBEnergyNointeraction, TBCharacterNointeraction} =
  Chop[CalculateBands[HNointeractionfun, KPoints]];
```

and plot the bands.

In[20]:=
```
CharacterPlotBandStructure[TBEnergyNointeraction, TBCharacterNointeraction,
 Knames, CharacterToColor, CharacterToThickness, -10, 30]
```

Out[20]=



How do we know that there are only four Eigen values at any given k-point ?

In[21]:=
```
HNointeractionfun[1, 0.5, 0]
```

Out[21]=
```
{{0.1 + 0. i, 0., 0., 0.}, {0., 4.1 + 0. i, 0., 0.},
 {0., 0., 8.1 + 0. i, 0.}, {0., 0., 0., 9. + 0. i}}
```

As a next step we include mixing between the s and p band

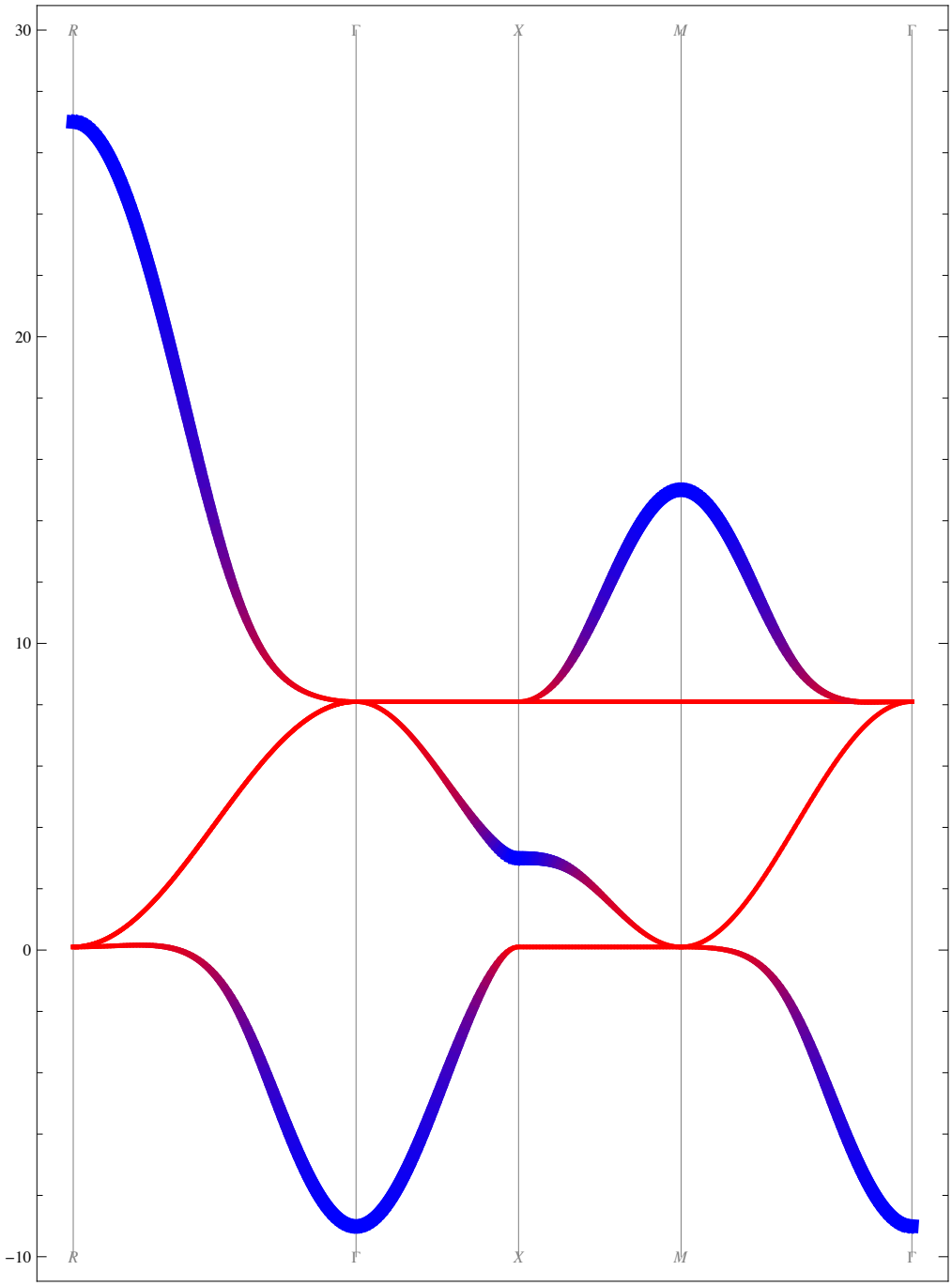
In[22]:=
```
ϵp = 4.1;
ϵs = 9;
ssσ = -3;
ppσ = 2;
spσ = 2;
Hfun[κx_, κy_, κz_] := Evaluate[N[H]];
```

and calculate the eigenstates.

In[28]:=
```
{TBEnergy, TBCharacter} = Chop[CalculateBands[Hfun, KPoints]];
```

In[29]:=
```
CharacterPlotBandStructure[TBEnergy, TBCharacter,
 Knames, CharacterToColor, CharacterToThickness, -10, 30]
```

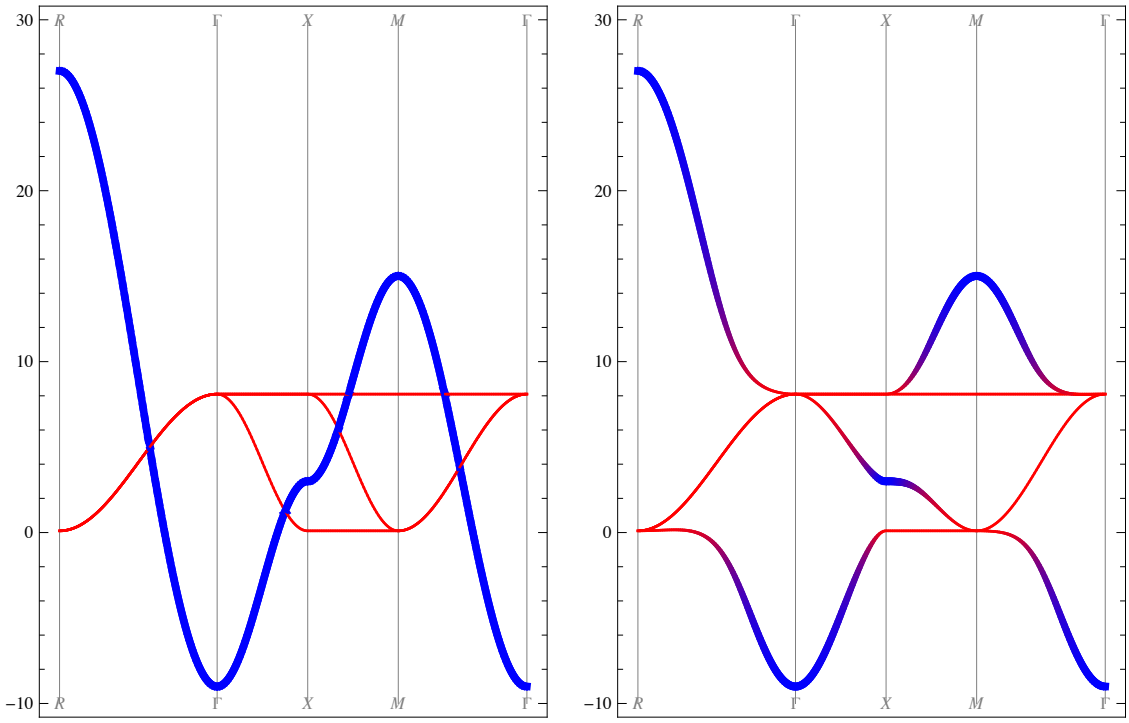
Out[29]=



And plot the band structure without (left) and with spin-orbit coupling (right).

In[30]:=
```
PltTBNoInt =
  CharacterPlotBandStructure[TBEnergyNointeraction, TBCharacterNointeraction,
   Knames, CharacterToColor, CharacterToThickness, -10, 30];
PltTB = CharacterPlotBandStructure[TBEnergy, TBCharacter,
   Knames, CharacterToColor, CharacterToThickness, -10, 30];
Show[GraphicsGrid[{{PltTBNoInt, PltTB}}]]
```

Out[32]=



In order to get a topological nontrivial state we need the entanglement between orbital and spin. This is realized by the relativistic spin-orbit coupling. Spin-orbit coupling can be included in a tight binding Hamiltonian by simply doubling the basis, i.e. adding a spin up and spin down orbital for each state in the original basis. Then the spin-orbit coupling Hamiltonian is given as:

In[33]:=
```
ClearAll[εs, εp, ssσ, spσ, ppσ, ζ]
```

In[34]:=
```
HSOC = ζ
```

$$\begin{pmatrix} 0 & \frac{i}{2} & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & \frac{i}{2} & 0 & 0 & 0 \\ -\frac{1}{2} & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} ;$$

In[35]:=
```
H = {{ϵp + ppσ (e^(i π κx) + e^(-i π κx)),  0,  0,  spσ (e^(i π κx) - e^(-i π κx))},
     {0,  ϵp + ppσ (e^(i π κy) + e^(-i π κy)),  0,  spσ (e^(i π κy) - e^(-i π κy))},
     {0,  0,  ϵp + ppσ (e^(i π κz) + e^(-i π κz)),  spσ (e^(i π κz) - e^(-i π κz))},
     {spσ (-e^(i π κx) + e^(-i π κx)),  spσ (-e^(i π κy) + e^(-i π κy)),  spσ (-e^(i π κz) + e^(-i π κz)),  ϵs + ssσ (e^(i π κx) + e^(-i π κx) + e^(i π κy) + e^(-i π κy) + e^(i π κz) + e^(-i π κz))}};
```

In[36]:=
```
HSOC[[1 ;; 4, 1 ;; 4]] += H;
HSOC[[5 ;; 8, 5 ;; 8]] += H;
```

Let's now add spin-orbit coupling to the original tight binding Hamiltonian: H + HSOC

In[38]:=
```
MatrixForm[FullSimplify[HSOC]]
```

$$\begin{pmatrix}
2\,\mathrm{pp}\sigma\cos(\pi\kappa x)+\epsilon p & \frac{i\zeta}{2} & 0 & 2i\,\mathrm{sp}\sigma\sin(\pi\kappa x) & 0 & 0 & -\frac{\zeta}{2} & 0\\
-\frac{1}{2}(i\zeta) & 2\,\mathrm{pp}\sigma\cos(\pi\kappa y)+\epsilon p & 0 & 2i\,\mathrm{sp}\sigma\sin(\pi\kappa y) & 0 & 0 & -\frac{1}{2}(i\zeta) & 0\\
0 & 0 & 2\,\mathrm{pp}\sigma\cos(\pi\kappa z)+\epsilon p & 2i\,\mathrm{sp}\sigma\sin(\pi\kappa z) & \frac{\zeta}{2} & \frac{i\zeta}{2} & 0 & 0\\
-2i\,\mathrm{sp}\sigma\sin(\pi\kappa x) & -2i\,\mathrm{sp}\sigma\sin(\pi\kappa y) & -2i\,\mathrm{sp}\sigma\sin(\pi\kappa z) & 2\,\mathrm{ss}\sigma(\cos(\pi\kappa x)+\cos(\pi\kappa y)+\cos(\pi\kappa z))+\epsilon s & 0 & 0 & 0 & 0\\
0 & 0 & \frac{\zeta}{2} & 0 & 2\,\mathrm{pp}\sigma\cos(\pi\kappa x)+\epsilon p & -\frac{1}{2}(i\zeta) & 0 & 2i\,\mathrm{sp}\sigma\sin(\pi\kappa x)\\
0 & 0 & -\frac{1}{2}(i\zeta) & 0 & \frac{i\zeta}{2} & 2\,\mathrm{pp}\sigma\cos(\pi\kappa y)+\epsilon p & 0 & 2i\,\mathrm{sp}\sigma\sin(\pi\kappa y)\\
-\frac{\zeta}{2} & \frac{i\zeta}{2} & 0 & 0 & 0 & 0 & 2\,\mathrm{pp}\sigma\cos(\pi\kappa z)+\epsilon p & 2i\,\mathrm{sp}\sigma\sin(\pi\kappa z)\\
0 & 0 & 0 & 0 & -2i\,\mathrm{sp}\sigma\sin(\pi\kappa x) & -2i\,\mathrm{sp}\sigma\sin(\pi\kappa y) & -2i\,\mathrm{sp}\sigma\sin(\pi\kappa z) & 2\,\mathrm{ss}\sigma(\cos(\pi\kappa x)+\cos(\pi\kappa y)+\cos(\pi\kappa z))+\epsilon s
\end{pmatrix}$$

Using the same input as above for the various onsite energies and hoppings, and additionally including the value for spin-orbit coupling constant, let's evaluate the Eigen values:

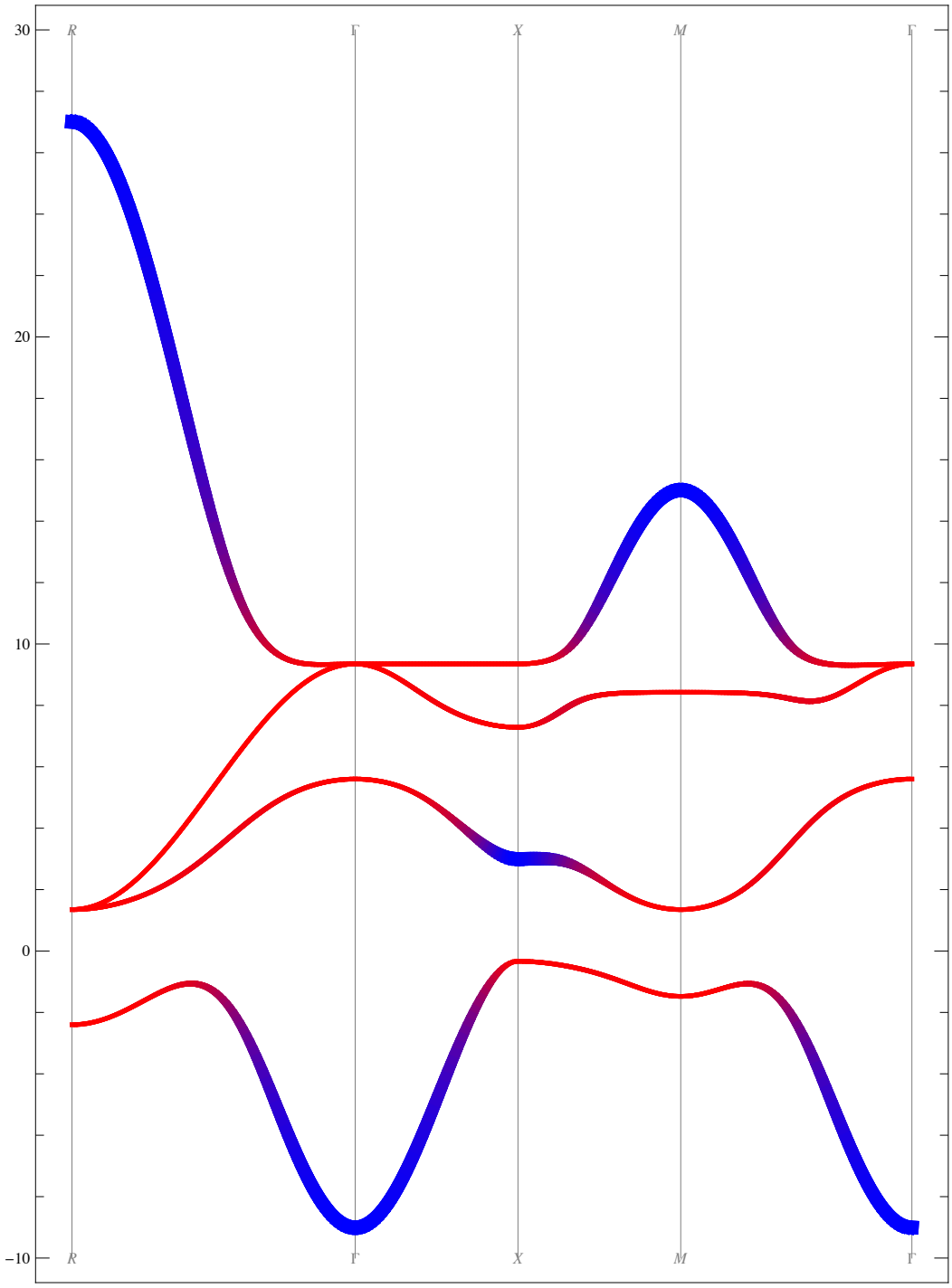
In[39]:=
```
ϵp = 4.1;
ϵs = 9;
ssσ = -3;
ppσ = 2;
spσ = 2;
ζ = 2.5;
HfunSOC[κx_, κy_, κz_] := Evaluate[N[HSOC]];
```

In[46]:=
```
{TBEnergySOC, TBCharacterSOC} = Chop[CalculateBands[HfunSOC, KPoints]];
```

Let's visualize it :

In[54]:=
```
CharacterPlotBandStructure[TBEnergySOC, TBCharacterSOC,
 Knames, CharacterToColorSOC, CharacterToThicknessSOC, -10, 30]
```

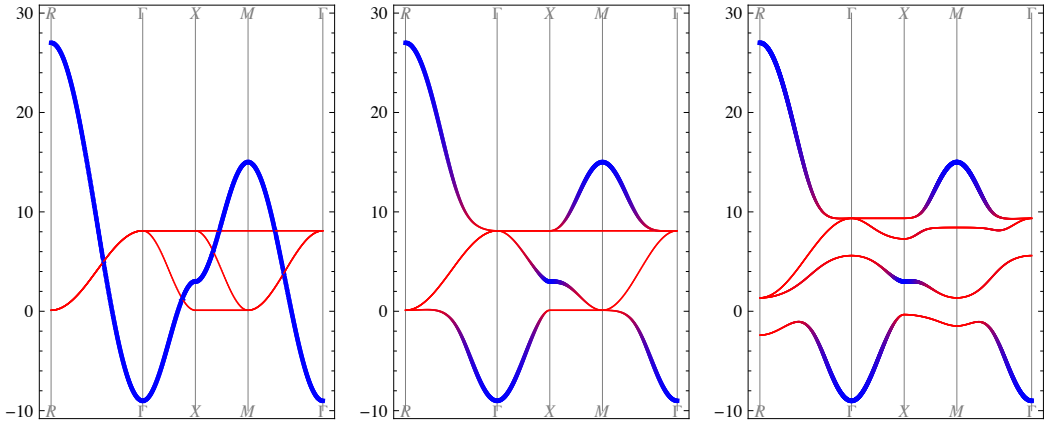
Out[54]=



Plotting all the graphs next to each other provides a complete picture

In[47]:=
```
PltTBNoInt =
 CharacterPlotBandStructure[TBEnergyNointeraction, TBCharacterNointeraction,
  Knames, CharacterToColor, CharacterToThickness, -10, 30];
PltTB = CharacterPlotBandStructure[TBEnergy, TBCharacter,
  Knames, CharacterToColor, CharacterToThickness, -10, 30];
PltTBSOC = CharacterPlotBandStructure[TBEnergySOC, TBCharacterSOC,
   Knames, CharacterToColorSOC, CharacterToThicknessSOC, -10, 30];
Show[GraphicsGrid[{{PltTBNoInt, PltTB, PltTBSOC}}]]
```

Out[49]=



One can see on the left: the s-p mixing creates hybridization gaps between the s and p band. However, at high symmetry points (R={1,1,1}, M={1,1,0}, X={1,0,0} and Γ={0,0,0}) the s and p band do not mix by symmetry. The system without spin-orbit coupling therefore is metallic. On the right we included spin-orbit coupling and this splits the p-bands into a j=1/2 and j=3/2 state. Now a single band splits off and if there is a filling of 2 electrons per site this band is fully occupied and the system is an insulator.

The gap, which is of indirect type (maximum of the valance band is at X, minimum of the conduction band at M or/and R) is between states of p character.

Topology

We now can test if the state with two electrons per site is a topological insulator or not. For cubic systems the number that distinguishes topological trivial case from a topological nontrivial case is calculated as the product of the parity of the occupied wave functions at Γ, X, M, and R. If +1, then the system is trivial and if -1, the system is topological.

We can make the following parity table

	s	p
Γ	1	-1
X	1	-1
M	1	-1
R	1	-1

Since we now consider an electron filling of 2, we only need to consider the parities of the single filled band. At Γ, the band is blue (s-orbital). Therefore the parity is +1. At X, p-character (red), therefore parity is -1. At M, p-character (red), parity is -1. At R, again p-character, parity is -1. So, we now need to take the product of these parities (+1 * -1 * -1 * -1). This gives a total of -1. Therefore, the system above is thus topological - non-trivial.