Srivani_HW6-Copy1

March 7, 2019

1 Srivani - Home work 6

In [1]:
```
from IPython.display import HTML

HTML('''<script>
code_show=true;
function code_toggle() {
 if (code_show){
 $('div.input').hide();
 } else {
 $('div.input').show();
 }
 code_show = !code_show
}
$( document ).ready(code_toggle);
</script>
<form action="javascript:code_toggle()"><input type="submit" value="Click here to toggl
```

Out[1]: <IPython.core.display.HTML object>

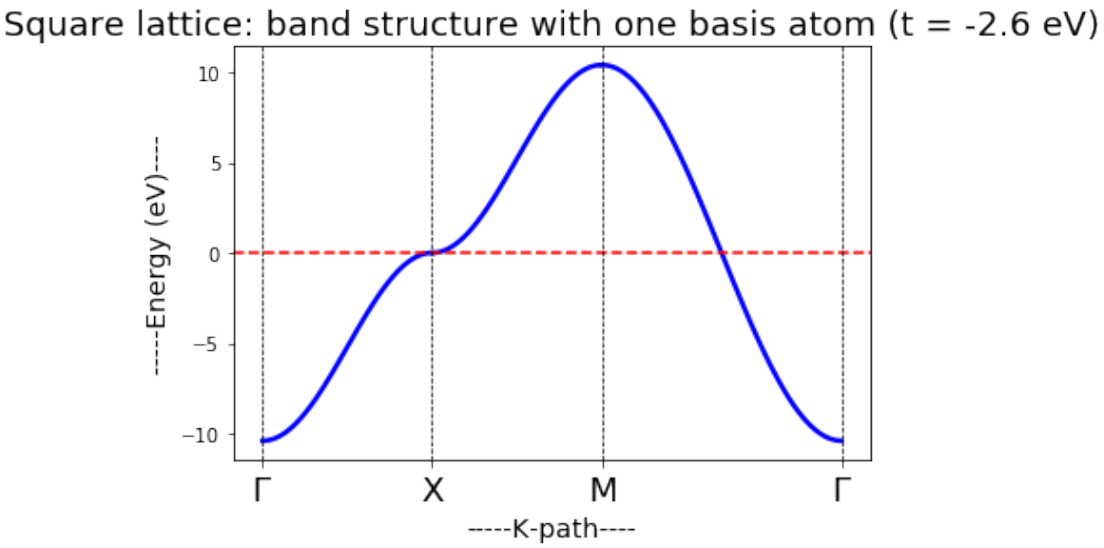
1.1 Repeat Homework 5 with square lattice

1.1.1 (a) Represent the bands along the symmtry lines :

$$\Gamma - X - M - \Gamma$$

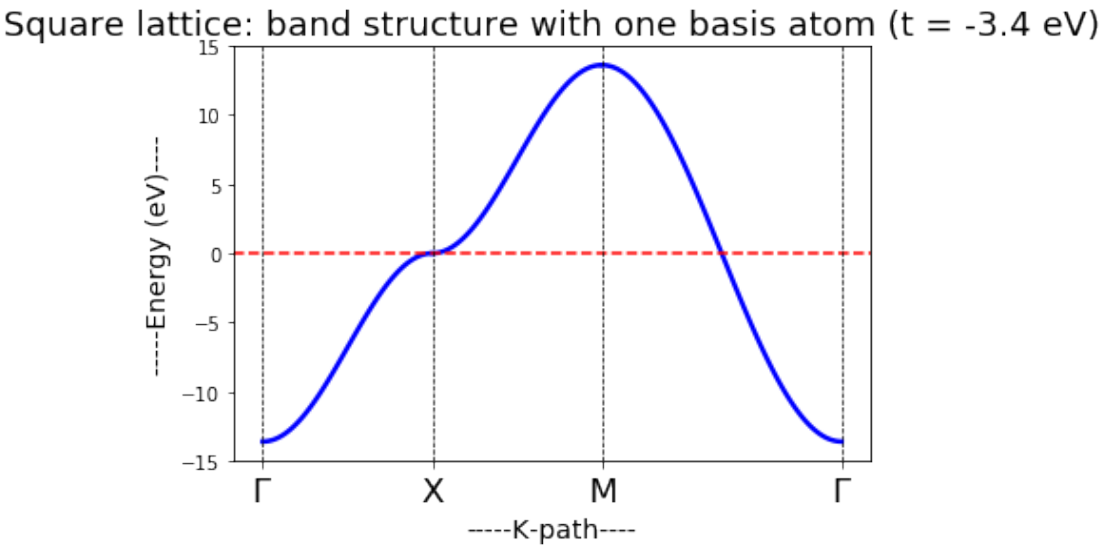
at t = -2.6 eV

In [2]:



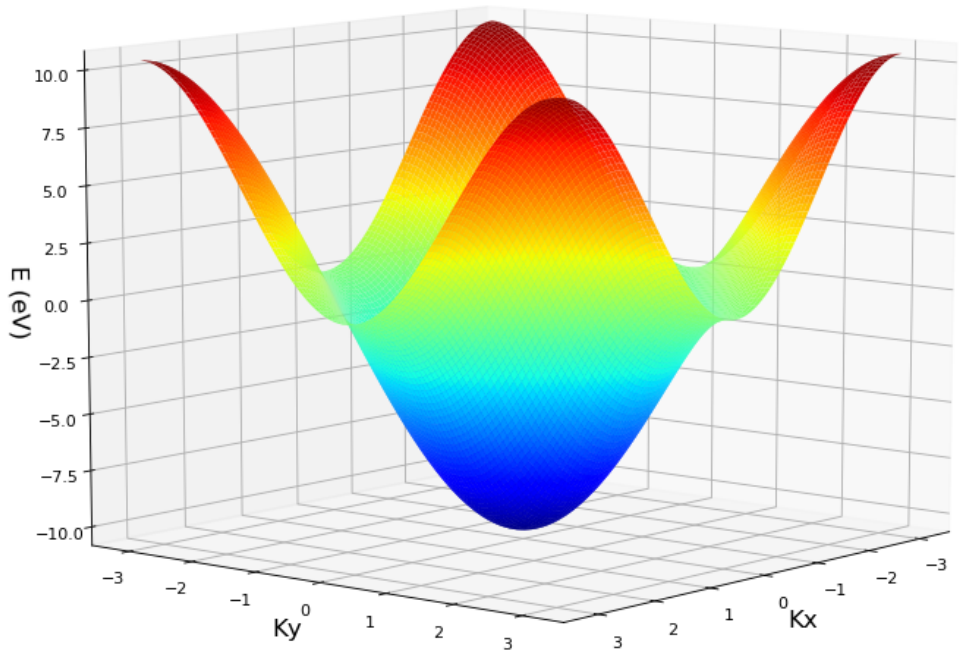
at t = -3.4 eV

In [3]:



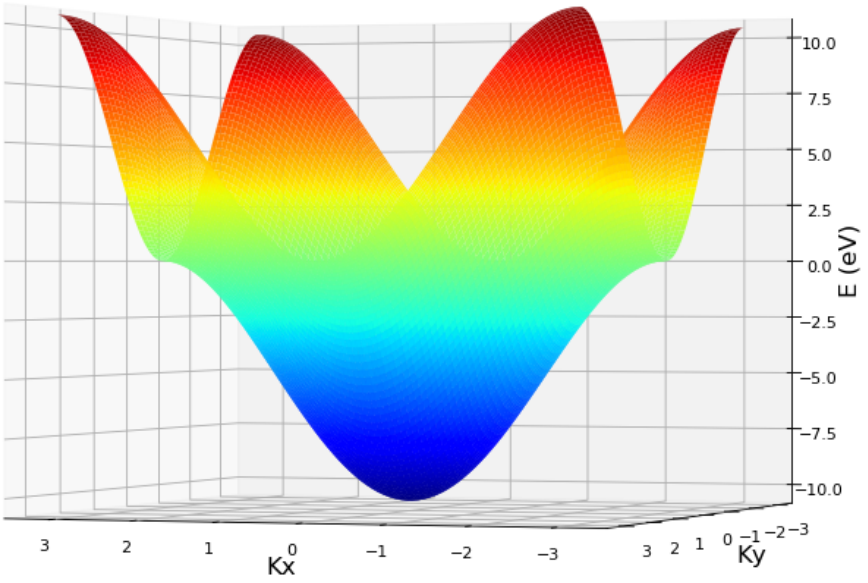
1.1.2 (b) Represent the bands as surface plots in the Brillouin zone.

In [3]:

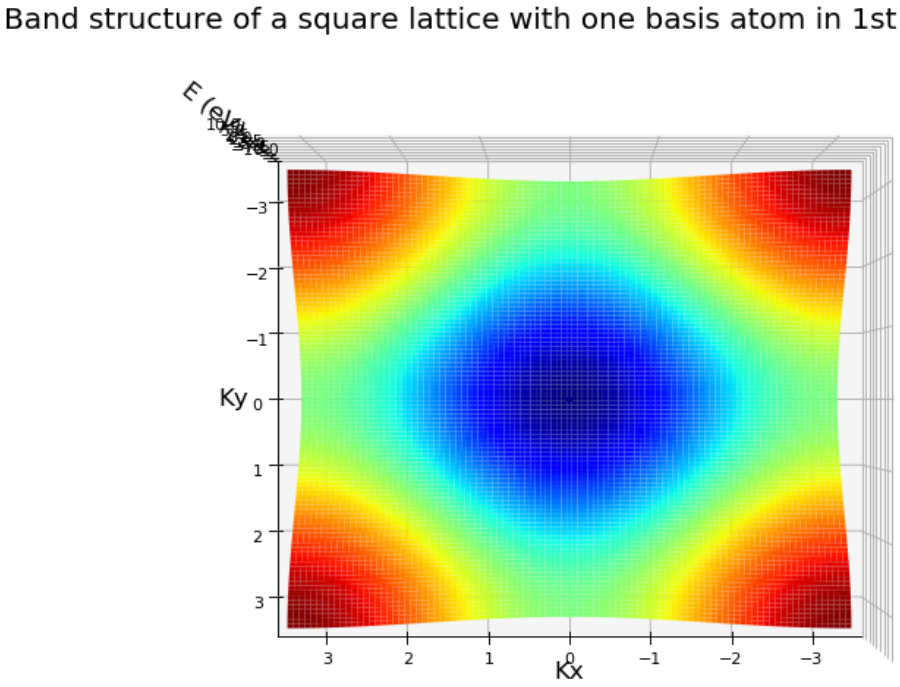

Band structure of a square lattice with one basis atom in 1st Brillouin zone
E (eV)
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
Ky
Kx
−3
−2
−1
0
1
2
3

In [6]:

Band structure of a square lattice with one basis atom in 1st Brillouin zone

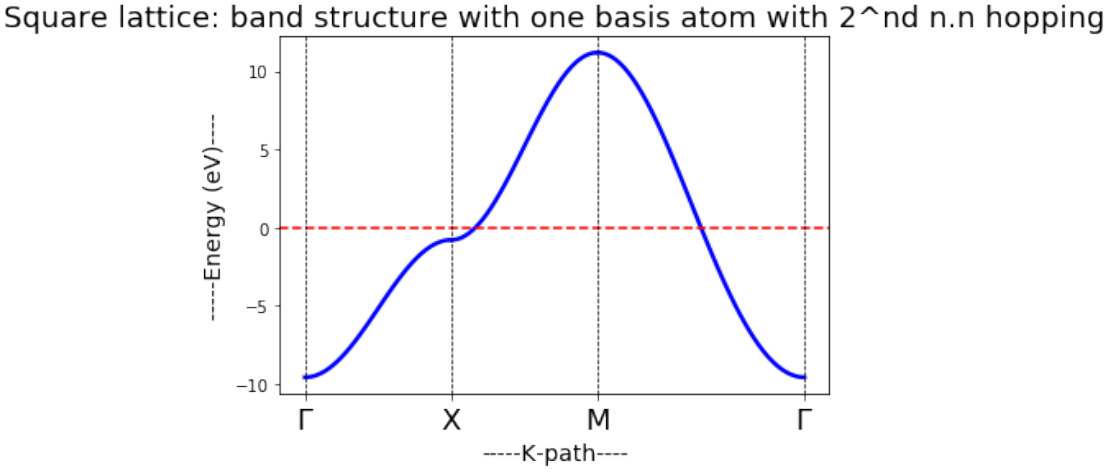


In [7]:



1.1.3 (c) Represent the bands considering an additional second nearest neighbor hopping term t=0.2eV and describe its effects.

In [3]:



1.1.4 (d) Represent the bands in the presence of VA=0.5 eV and VB=0.5 eV site potential differences.

There is only one basis atom in the primitive cell.

1.2 Problem 2: Pybinding

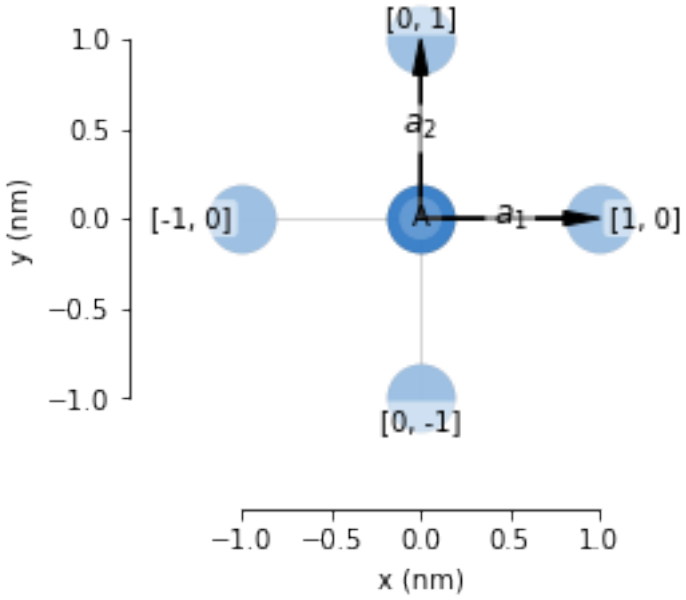
1.2.1 (a) Represent the bands along the symmtry lines :

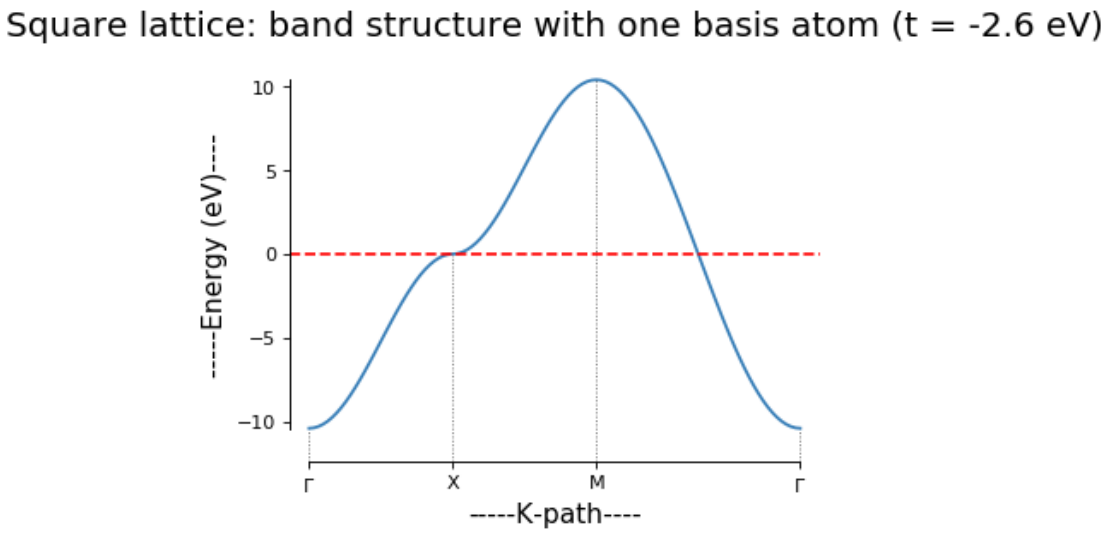
$$\Gamma - X - M - \Gamma$$

at t = -2.6 eV

In [16]:

Out[16]: Text(0.5,1,'Square lattice: band structure with one basis atom (t = -2.6 eV)')

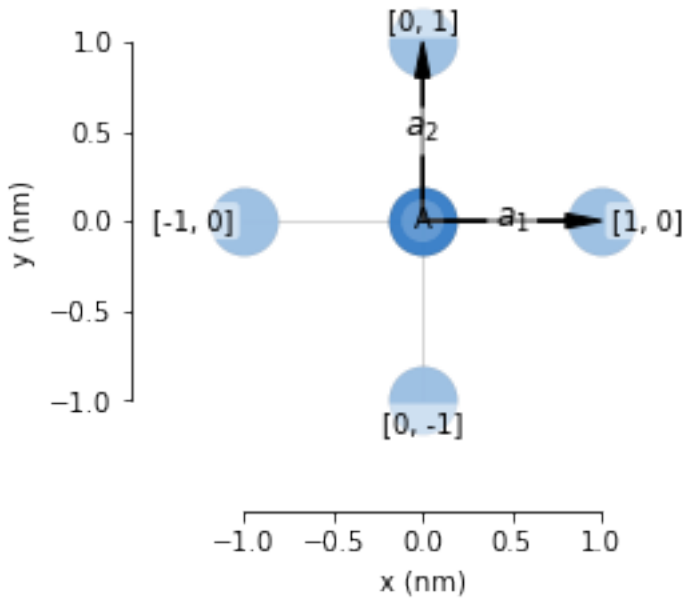


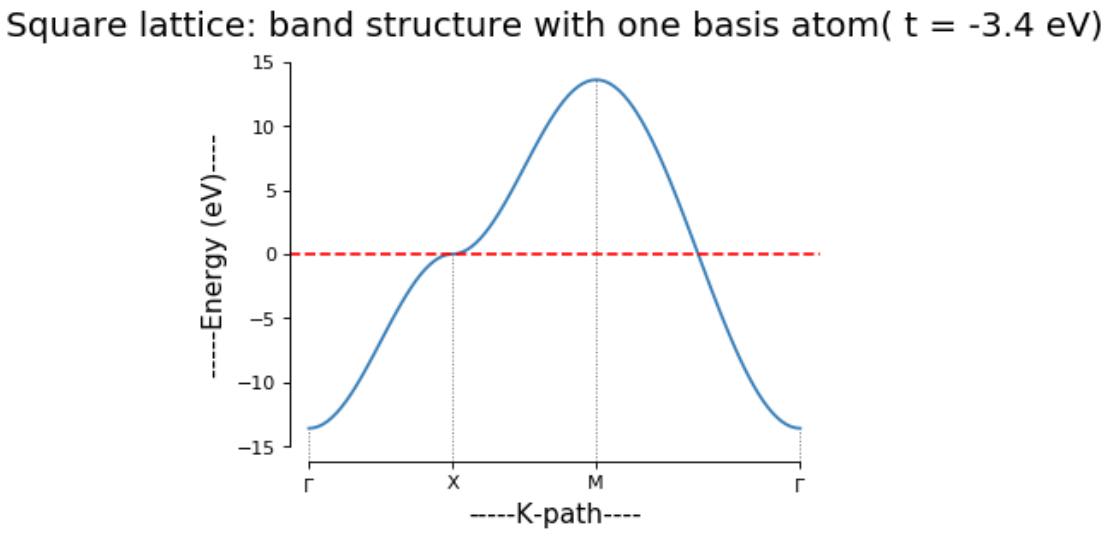


at t = -3.4 eV

In [17]:

Out[17]: Text(0.5,1,'Square lattice: band structure with one basis atom(t = -3.4 eV)')

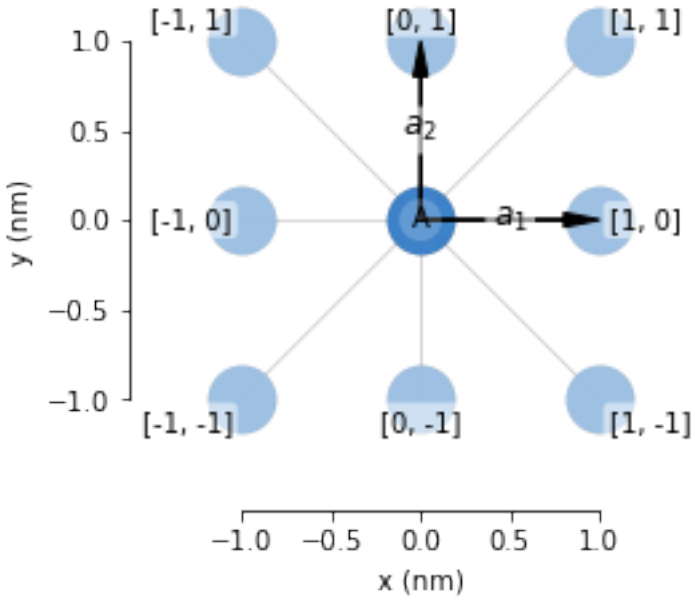




1.2.2 (c) Represent the bands considering an additional second nearest neighbor hopping term t=0.2 and describe its effects.

In [18]:

Out[18]: Text(0.5,1,'Square lattice: band structure with one basis atom with 2^nd n.n hopping')



Square lattice: band structure with one basis atom with 2^nd n.n hopping