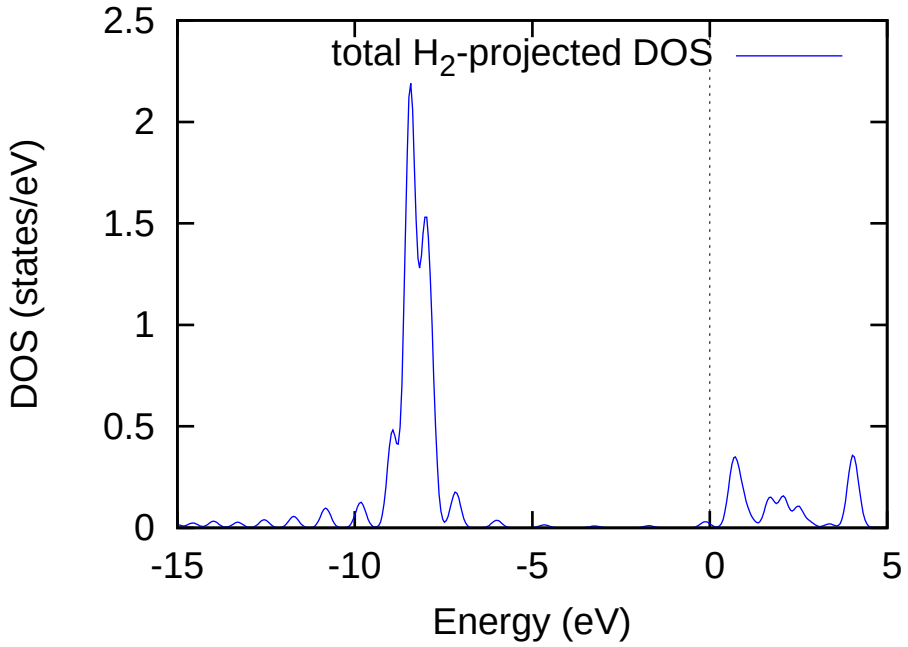
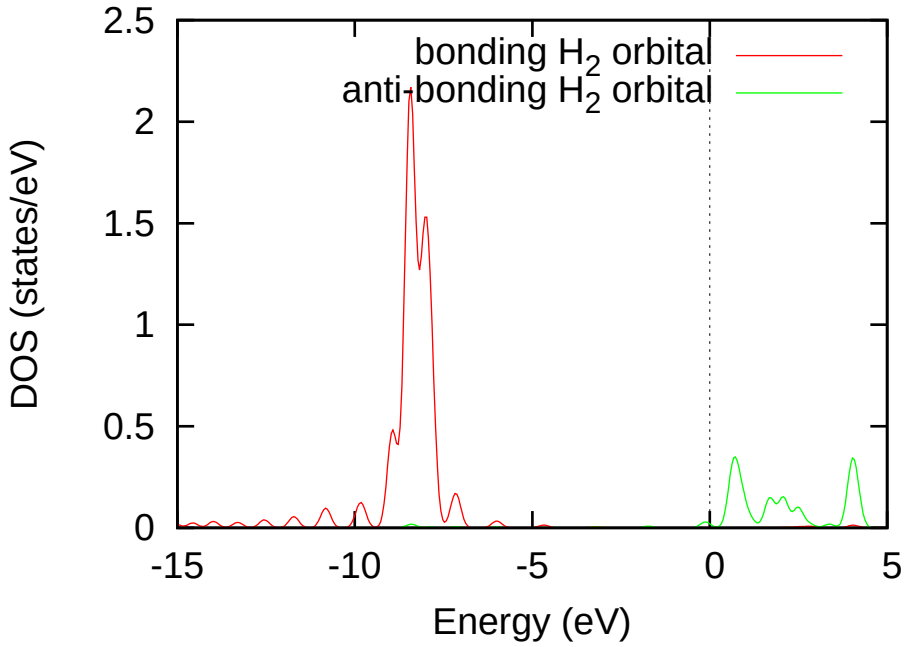
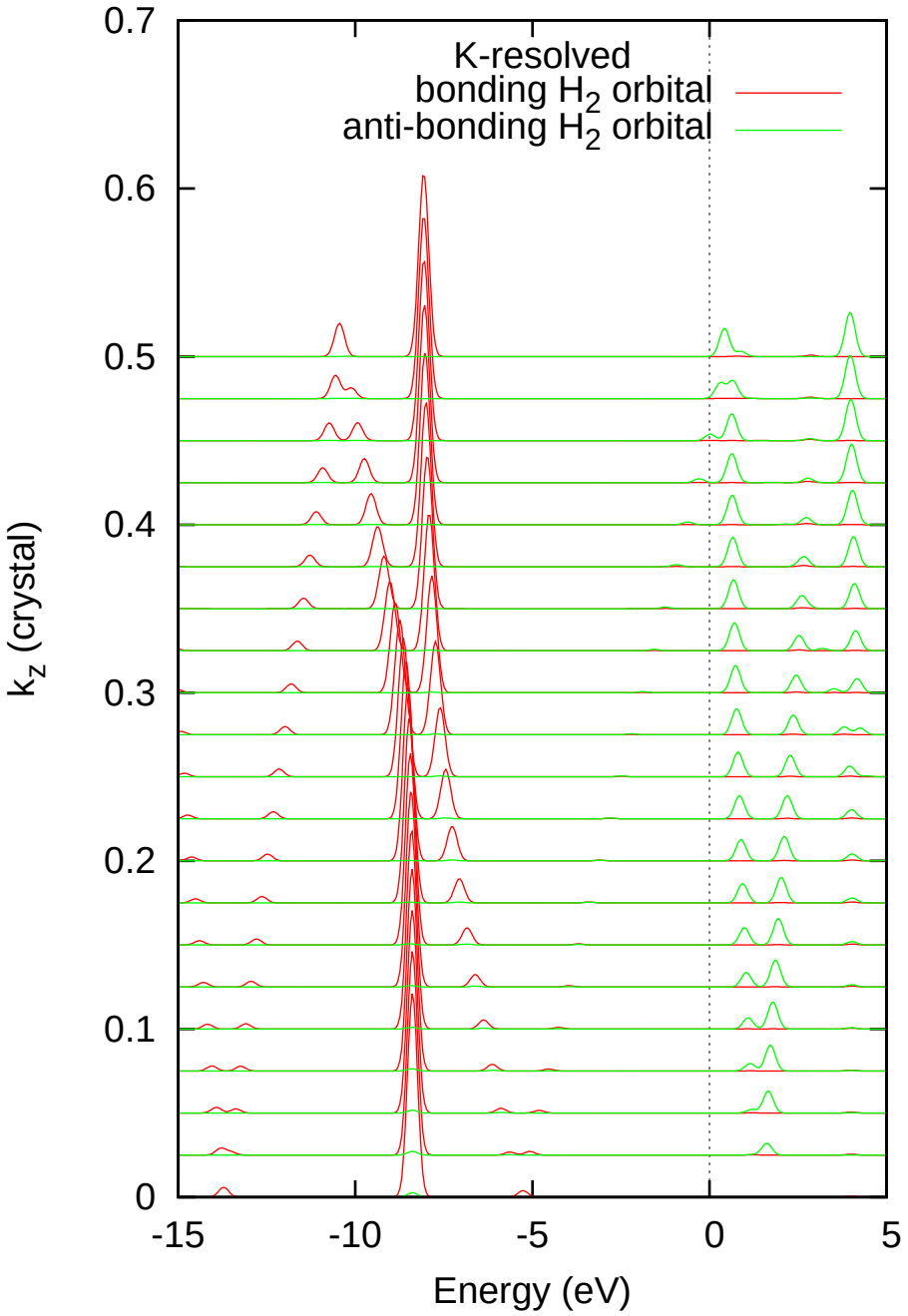

total H_2-projected DOS
DOS (states/eV)
Energy (eV)
2.5
2
1.5
1
0.5
0
-15
-10
-5
0
5


bonding H_2 orbital
anti-bonding H_2 orbital
DOS (states/eV)
Energy (eV)
2.5
2
1.5
1
0.5
0
-15
-10
-5
0
5


K-resolved
bonding H_2 orbital
anti-bonding H_2 orbital
k_z (crystal)
Energy (eV)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-15
-10
-5
0
5