In[●]:=

In[●]:= `Charting`$InteractiveHighlighting = False`

Out[●]=

False

In[●]:= `dat1 = Import[`
`    "/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM`
`      MANO/Computational material physics /Cluster`
`      data/P2/outputO2/outputETOT.csv", "Table"] // Flatten`

Out[●]=

{24.4871, -6.15164, -9.83918, -8.4155, -6.39093, -4.68474, -4.23425,
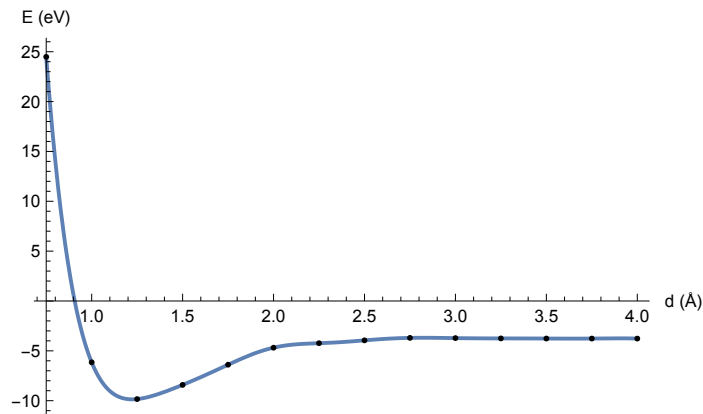 -3.94909, -3.70156, -3.72284, -3.75421, -3.76573, -3.76886, -3.77241}

In[●]:= `dattr = Transpose[{Range[0.75, 4, 0.25], dat1}]`

Out[●]=

{{0.75, 24.4871}, {1., -6.15164}, {1.25, -9.83918},
 {1.5, -8.4155}, {1.75, -6.39093}, {2., -4.68474}, {2.25, -4.23425},
 {2.5, -3.94909}, {2.75, -3.70156}, {3., -3.72284},
 {3.25, -3.75421}, {3.5, -3.76573}, {3.75, -3.76886}, {4., -3.77241}}

In[●]:= `plt = Plot[Interpolation[dattr, Method → "Spline", InterpolationOrder → 6][x],`
`    {x, 0.75, 4}, Epilog → {Point[dattr]},`
`    PlotRange → All, AxesLabel → {"d (Å)", "E (eV)"}]`

Out[●]=

In[●]:= `Export["/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM`
`      MANO/Computational material physics /Lab reports/2/inplt.pdf", plt]`

Out[●]=

/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
  MANO/Computational material physics /Lab reports/2/inplt.pdf

```
In[ ]:= eoccs = Import[
         "/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
           MANO/Computational material physics /Cluster
           data/P2/outputO2/eOccs.tsv", "Table"]
```

```
Out[ ]=
      {{1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
       {1., 1., 1., 0.5, 0.5, 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
       {1., 1., 1., 0.5, 0.5, 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
       {1., 1., 1., 0.5, 0.5, 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
       {1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
       {1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
       {1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
       {1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0.},
       {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
       {1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0.}}
```

In[•]:= **upoccs = eoccs[[1 ;; ;; 2]]**

Out[•]=
```
{{1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.},
 {1., 1., 1., 1., 1., 1., 1., 1., 0., 0., 0.}}
```
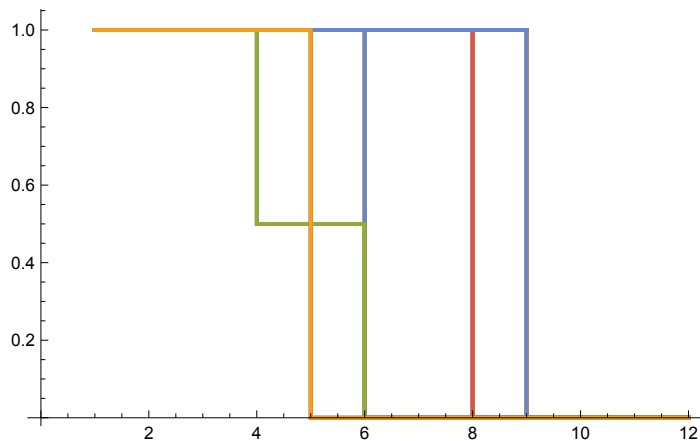
In[•]:= **downoccs = eoccs[[2 ;; ;; 2]]**

Out[•]=
```
{{1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 0.5, 0.5, 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 0.5, 0.5, 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 0.5, 0.5, 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0.},
 {1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0.}}
```

In[•]:= **ListStepPlot[eoccs]**

Out[•]=

```
In[•]:= evals = Import[ToString@StringForm["/Users/giovannigravili/Library/Mobile
            Documents/com~apple~CloudDocs/LM
            MANO/Computational material physics /Cluster
            data/P2/outputO2/output``.csv", #], "Table"] & /@ {"Up", "Down"};
```

```
In[•]:= ev1 = First@evals // Transpose;
```

```
In[•]:= ev1〚1〛 // Length
```
```
Out[•]=
        14
```

```
In[•]:= Range[0.75, 4, 0.25] // Length
```
```
Out[•]=
        14
```
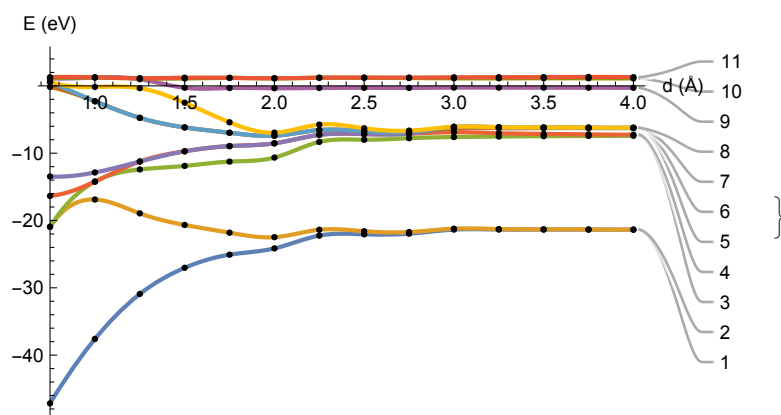
```
In[•]:= Length@evals
```
```
Out[•]=
        2
```

```
In[•]:= af = Table[Transpose[{Range[0.75, 4, 0.25], #}] & /@ Transpose[f], {f, evals}];
```

```
In[•]:= pll =
        Table[Magnify[Plot[Interpolation[#, Method → "Spline"][x] & /@ afi // Evaluate,
            {x, 0.75, 4}, ImageSize → Medium, Epilog → {Point[#] & /@ afi},
            AxesLabel → {"d (Å)", "E (eV)"}, PlotLabels → Range[1, 11]], 1.1], {afi, af}]
```
```
Out[•]=
```
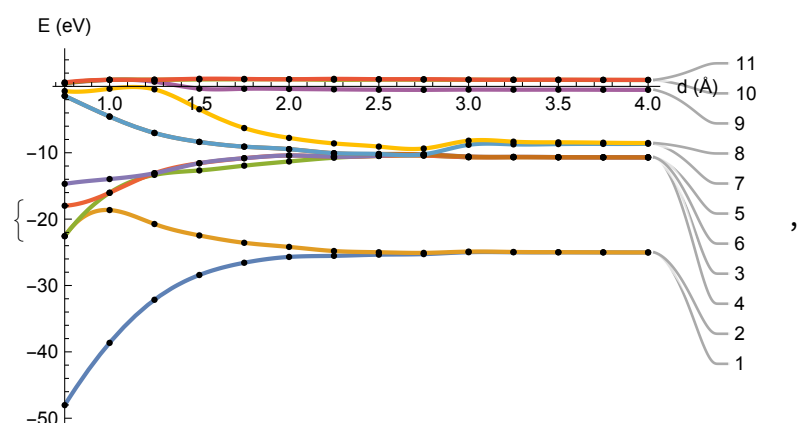
```
In[ ]:= Export[ToString@StringForm[
          "/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
            MANO/Computational material physics /Lab reports/2/pllddep``.pdf",
          #2], #1] & @@@ Transpose[{pll, {"Up", "Down"}}]

Out[ ]=
      {/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
        MANO/Computational material physics /Lab reports/2/pllddepUp.pdf,
       /Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
        MANO/Computational material physics /Lab reports/2/pllddepDown.pdf}
```

```
In[ ]:= g = Grid[Transpose@#, Frame → All] & /@ evals
```

Out[ ]=

−48.	−38.	−32.	−28.	−26.	−25.	−25.	−25.	−25.	−24.	−24.	−25.	−25.	−25.
.	.	.	.	.	.	.	.	.	.	.	.	.	.
0	6	1	4	5	6	5	3	2	9	9	0	0	0
2	4	5	2	7	9	3	5	7	8	9	0	1	2
7	6	1	0	4	5	5	6	2	3	2	4	4	2
1	4	8	5	4	4	5	9	3	8	9	5	3	7
−22.	−18.	−20.	−22.	−23.	−24.	−24.	−24.	−25.	−24.	−24.	−24.	−25.	−25.
.	.	.	.	.	.	.	.	.	.	.	.	.	.
5	6	7	4	5	1	8	9	0	8	9	9	0	0
6	3	3	6	6	8	0	9	8	9	4	8	0	1
5	4	6	1	8	5	6	1	6	5	7	1	3	6
7		7	1	6	5	4	3	8	4	9		4	2
−22.	−16.	−13.	−12.	−11.	−11.	−10.	−10.	−10.	−10.	−10.	−10.	−10.	−10.
.	.	.	.	.	.	.	.	.	.	.	.	.	.
5	0	3	6	9	3	7	4	4	6	6	6	6	7
6	3	3	6	4	1	5	8	2	7	8	8	9	0
5	2	2	7	8	3	3	3	5	1		9	7	3
7	9		1		6	2	3	9	2		4	4	6
−17.	−16.	−13.	−11.	−10.	−10.	−10.	−10.	−10.	−10.	−10.	−10.	−10.	−10.
.	.	.	.	.	.	.	.	.	.	.	.	.	.
9	0	0	5	8	4	5	4	4	6	6	6	6	7
8	3	8	8	2	1	8	8	2	7	8	8	9	0
6	2	5	0	0	5	9	3	5	1		9	7	3
5	9	7	2	3	3	2	3	9	2		4	4	6
−14.	−13.	−13.	−11.	−10.	−10.	−10.	−10.	−10.	−10.	−10.	−10.	−10.	−10.
.	.	.	.	.	.	.	.	.	.	.	.	.	.
6	9	0	5	8	4	5	4	2	5	6	6	6	6
8	6	8	8	2	1	8	4	5	7	2	5	7	9
3	2	5	0	0	5	9	6	6	8	6	7	8	2
5	1	7	2	3	3	2	3	8	8		3	9	1
−1..	−4..	−7..	−8..	−9..	−9..	−10.	−10.	−10.	−10.	−10.	−10.	−10.	−10.
4	5	0	3	0	4	.	.	.	.	.	.	.	.
3	5	1	6	8	5	0	1	2	5	6	6	6	6
4	0	8	5	2	4	6	8	5	7	2	5	7	9
5	1	8	1	9	8	7	8	6	8	6	7	8	2

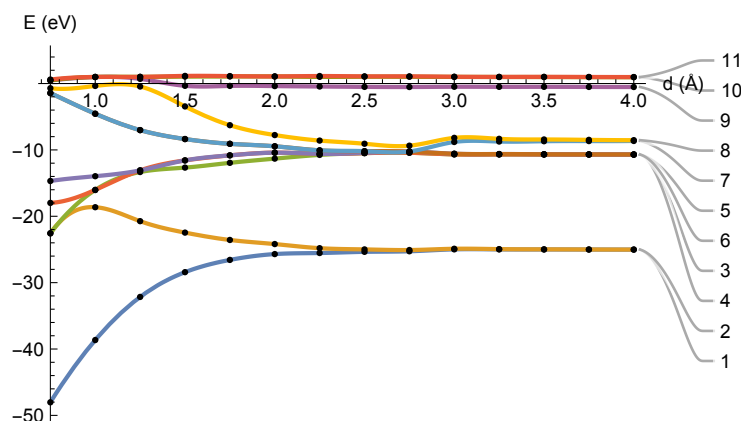|						7	6	8	8		3	9	1
−1.4345	−4.5501	−7.0188	−8.3651	−9.0829	−9.4548	−10.0677	−10.1886	−10.2332	−8.8054	−8.7376	−8.6918	−8.6684	−8.6496
−0.7053	−0.3613	−0.4467	−3.4485	−6.2769	−7.7641	−8.5949	−9.0762	−9.3639	−8.1849	−8.3315	−8.4289	−8.4876	−8.5325
0.4701	0.9817	0.7003	−0.3435	−0.3598	−0.3858	−0.4449	−0.5039	−0.5225	−0.4856	−0.4989	−0.4953	−0.5104	−0.5224
0.4701	0.9902	1.0048	1.0516	1.0689	1.0672	1.011	1.0303	1.0212	1.0008	0.9868	0.9793	0.9663	0.9555
0.6012	0.9902	1.0048	1.1474	1.12	1.0727	1.1298	1.0837	1.0832	1.022	0.998	1.0043	0.9886	0.9778

```
In[ ]:= h = Column[{#3, Spacer[1], Row[{Spacer[225], #1, Spacer[50], #2}]}] & @@@
          Transpose[{mat, pll, g}]
```

Out[ ]=

−48.0271	−38.6464	−32.1518	−28.4205	−26.5744	−25.6954	−25.5355	−25.3569	−25.2723	−24.9938	−24.9929	−25.0045	−25.0143	−25.0227
−22.5657	−18.6344	−20.7367	−22.4611	−23.5686	−24.1855	−24.8064	−24.9913	−25.0868	−24.8954	−24.9479	−24.9814	−25.0034	−25.0162
−22.5657	−16.0329	−13.3322	−12.6671	−11.9481	−11.3136	−10.7532	−10.4833	−10.4259	−10.6712	−10.68	−10.6894	−10.6974	−10.7036
−17.98	−16.03	−13.08	−11.58	−10.82	−10.41	−10.58	−10.48	−10.42	−10.67	−10.68	−10.68	−10.69	−10.70

6.5	2.9	5.7	0.2	0.3	5.3	9.2	3.3	5.9	1.2		9.4	7.4	3.6
−14.6835	−13.9621	−13.0857	−11.5802	−10.8203	−10.4153	−10.5892	−10.4463	−10.2578	−10.5788	−10.626	−10.6573	−10.6789	−10.6921
−1.4345	−4.5501	−7.0188	−8.3651	−9.0829	−9.4548	−10.0677	−10.1886	−10.2568	−10.5788	−10.626	−10.6573	−10.6789	−10.6921
−1.4345	−4.5501	−7.0188	−8.3651	−9.0829	−9.4548	−10.0677	−10.1886	−10.2532	−8.8054	−8.7376	−8.6918	−8.6684	−8.6496
−0.7053	−0.3613	−0.4467	−3.4485	−6.2769	−7.7641	−8.5949	−9.072	−9.3639	−8.1849	−8.3315	−8.4289	−8.4876	−8.5325
0.4701	0.9817	0.7003	−0.3435	−0.3598	−0.3858	−0.449	−0.5036	−0.5227	−0.4857	−0.4986	−0.4953	−0.5104	−0.5224
0.4701	0.9902	1.0048	1.0516	1.0689	1.0672	1.011	1.0303	1.0212	1.0008	0.9868	0.9793	0.9663	0.9555
0.6012	0.9902	1.0048	1.1474	1.12	1.0727	1.1298	1.0837	1.0832	1.022	0.998	1.0043	0.9886	0.9778

1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1
0	0	0	0	0	0	1	1	1	1	1	1	1	1
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

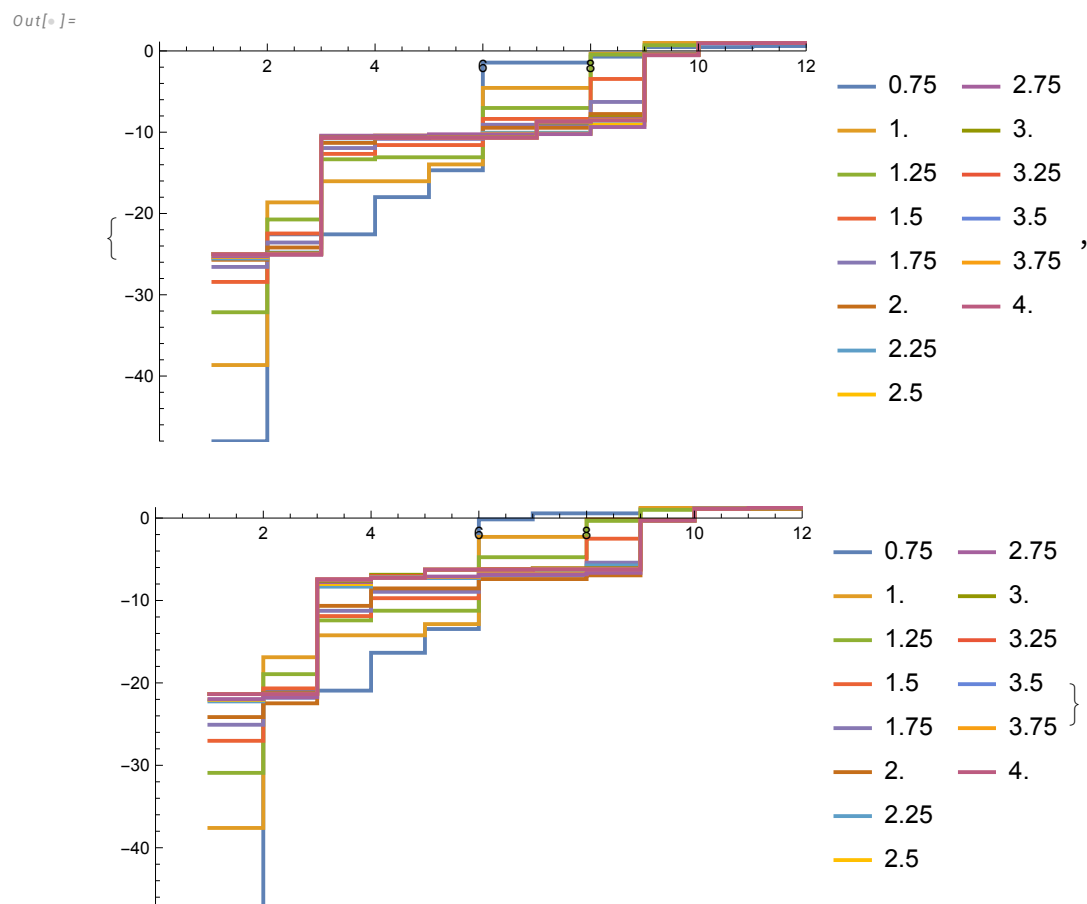*In[ ]:=* **Export[ToString@StringForm[**
      "/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
        MANO/Computational material physics /Lab reports/2/pllddep``.pdf",
      #2], Magnify[#1, 0.7]] &@@@ Transpose[{h, {"Up", "Down"}}]

Out[ ]=

      {/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
        MANO/Computational material physics /Lab reports/2/pllddepUp.pdf,
      /Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
        MANO/Computational material physics /Lab reports/2/pllddepDown.pdf}

In[ ]:= **ListStepPlot[# // Evaluate,**
      PlotLegends → Range[0.75, 4, 0.25], ImageSize → Medium] & /@ evals

Out[ ]=

In[ ]:= `v = SparseArray@Transpose@Rationalize[eoccs]`

Out[ ]=

SparseArray[⊞ 〜 Specified elements: 171 / Dimensions: {11, 28}]

In[ ]:= `Grid[v]`

Out[ ]=

```
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 ½ 1 ½ 1 ½ 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 ½ 1 ½ 1 ½ 1 0 1 0 1 0 1 0 1 0
1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0
1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0
0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

In[ ]:= `MatrixPlot[v]`

Out[ ]=
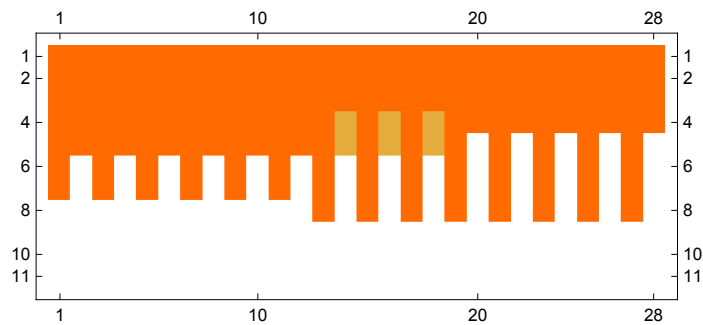
In[ ]:= `mat = Grid[Transpose[#] // Rationalize, Frame → All] & /@ {upoccs, downoccs}`

Out[ ]=

```
In[ ]:= Export[ToString@StringForm[
          "/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
            MANO/Computational material physics /Lab reports/2/occsTab``.pdf",
          #2], #1] & @@@ Transpose[{mat, {"Up", "Down"}}]

Out[ ]= {/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
          MANO/Computational material physics /Lab reports/2/occsTabUp.pdf,
         /Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
          MANO/Computational material physics /Lab reports/2/occsTabDown.pdf}

In[ ]:= ListStepPlot[#, PlotLegends → Range[0.75, 4, 0.25], PlotRange → {-0.1, All}] & /@
         eoccs;

In[ ]:= Export["/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
          MANO/Computational material physics /Lab reports/2/occsTab.pdf", mat]

Out[ ]= /Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
          MANO/Computational material physics /Lab reports/2/occsTab.pdf

In[ ]:= ArrayPlot@Transpose@eoccs // Export["", #] &

        ⚠ Export : First argument "" is not a valid file specification.    ⓘ

Out[ ]= $Failed

In[ ]:= Export["/Users/giovannigravili/Library/Mobile
          Documents/com~apple~CloudDocs/LM MANO/Computational
          material physics /Lab reports/2/occsMat.pdf", MatrixPlot[v]]

Out[ ]= /Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
          MANO/Computational material physics /Lab reports/2/occsMat.pdf
```

Part 2 molecules

```
In[1]:= data =
         Dataset[Import[ToString@StringForm["/Users/giovannigravili/Library/Mobile
                 Documents/com~apple~CloudDocs/LM
                 MANO/Computational material physics /Cluster
                 data/P2/potfit/outputETOT``.csv", #], "Table",
             "HeaderLines" → 0, "FieldSeparators" → "\t", "NumberPoint" → ".",
             CharacterEncoding → "UTF8"]][All, Range[1, 1]]][All,
           Rule @@@ Transpose[{ToString@StringForm["Band ``", #] & /@ Range[1, 1] //
               Evaluate, Range[1, 1]}] // Association] & /@ {"o2", "co", "no"};

In[2]:= data2 = Transpose[{Apply[Range, #2], #1[All, ToString@StringForm["Band 1"]]} //
             Normal // Evaluate] & @@@ Transpose[
           {data, {{1.08, 1.32, 0.024}, {1.02, 1.24, 0.022}, {1.03, 1.27, 0.024}}}];
```

In[3]:= `Range[1.08, 1.32, 0.024 ] // Length`

Out[3]= `11`

In[4]:= `j = {5, 5, 5};`

In[5]:= `ip = Table[`
`        Interpolation[di, InterpolationOrder → 5, Method → "Spline"], {di, data2}];`

In[6]:= `fits = Fit[#, {1, x, x^2}, x] & /@ (Take[#1, {#2, -1}] & @@@ Transpose[{data2, j}])`

Out[6]= $\{42.0008 - 81.7954\,x + 32.9733\,x^2,$
$\quad 45.9296 - 106.08\,x + 46.3356\,x^2, 45.7045 - 98.2047\,x + 41.8319\,x^2\}$

In[7]:= `Factor /@ fits`

Out[7]= $\{32.9733\,(-1.75475 + 1.\,x)\,(-0.725906 + 1.\,x),$
$\quad 46.3356\,(-1.70957 + 1.\,x)\,(-0.579817 + 1.\,x),$
$\quad 41.8319\,(-1.70787 + 1.\,x)\,(-0.639729 + 1.\,x)\}$

In[8]:= `coeffs = Fit[#, {1, x, x^2}, x, "BestFitParameters"] & /@`
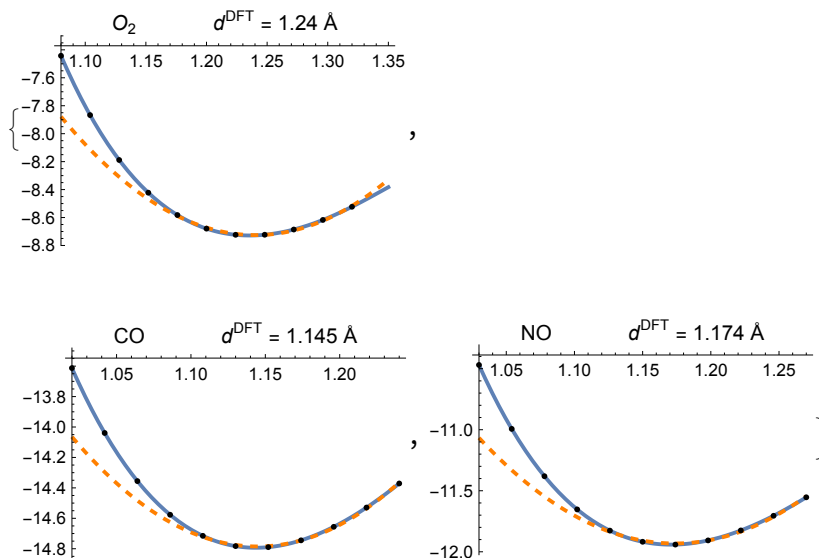`        (Take[#1, {#2, -1}] & @@@ Transpose[{data2, j}]);`

In[9]:= `mins = Round[FindMinimum[#, {x, 1.25}, AccuracyGoal → 3][[2]][[1]][[2]] & /@ fits, 0.001]`

Out[9]= $\{1.24, 1.145, 1.174\}$

In[10]:= `fpl =`
`    Show[Plot[#1[d], {d, #3[[1]], #3[[2]]}, ImageSize → 200, Epilog → {Point[#] & /@ #2},`
`        PlotRange → All], Plot[#4, {x, #3[[1]], #3[[2]]}, PlotStyle → {Orange, Dashed},`
`   PlotRange → All], PlotLabel → StringForm["``\t d`$^{DFT}$` = `` Å", #5, #6]] & @@@`
`    Transpose[{ip, data2, {{1.08, 1.35}, {1.02, 1.24}, {1.03, 1.27}},`
`        fits, {"O`$_2$`", "CO", "NO"}, mins}]`

Out[10]=

In[11]:= `expmins = {1.201, 1.128, 1.151};`

$\dfrac{\text{\#1} - \text{\#2}}{\text{\#2}}$ `& @@@ Transpose[{mins, expmins}] // PercentForm`

Out[12]//PercentForm=

`{3.247%, 1.507%, 1.998%}`

In[13]:= `Export["/Users/giovannigravili/Library/Mobile`
`    Documents/com~apple~CloudDocs/LM MANO/Computational`
`    material physics /Lab reports/2/fitpltssss.pdf", Row[fpl]]`

Out[13]=

`/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM`
`    MANO/Computational material physics /Lab reports/2/fitpltssss.pdf`

In[14]:= `Around[1.151, 1.151 / 10]`

Out[14]=

`1.15 ± 0.12`

In[15]:= `Range[1.15 - 0.12, 1.15 + 0.12, 0.24 / 10]`

Out[15]=

`{1.03, 1.054, 1.078, 1.102, 1.126, 1.15, 1.174, 1.198, 1.222, 1.246, 1.27}`

In[16]:= `% // Length`

Out[16]=

`11`

In[17]:= `0.24 / 10`

Out[17]=

`0.024`

In[18]:= `f = NonlinearModelFit`$\Big[$`With[{b = RandomReal[{0, 3}, 3500]},`

`    Transpose[{b, Table[#, {x, b}]}]],` $\dfrac{k}{2}$ $(x - x0)^2 + h, \{k, x0, h\}, x\Big]$ `& /@ fits`

Out[18]=

$\Big\{$ `FittedModel`$\Big[$ $-8.72571 + 32.9733\,(-1.24033 + x)^2$ $\Big]$,

`FittedModel`$\Big[$ $-14.785 + 46.3356\,(-1.14469 + x)^2$ $\Big]$ `, FittedModel`$\Big[$ $-11.9318 + 41.8319\,(-1.1738 + x)^2$ $\Big]\Big\}$

In[19]:= `ks = Quantity`$\Big[$ $\dfrac{1}{10^{-20}}$ `#["BestFitParameters"]〚1〛〚2〛 & /@ f,` $\dfrac{\text{"Electronvolts"}}{\text{"Meters"}^2}$ $\Big]$ `//`

`    UnitConvert[#, "SIBase"] &`

Out[19]=

$\Big\{$ $1056.58\ \text{kg}/\text{s}^2$, $1484.76\ \text{kg}/\text{s}^2$, $1340.44\ \text{kg}/\text{s}^2$ $\Big\}$

In[20]:= `Quantity[1, "Meters" / "Seconds"]`

Out[20]=

$1\ \text{m}/\text{s}$

In[21]:=

In[22]:= `RandomReal[{1, 3}, 15]`

Out[22]=

{2.86051, 1.07924, 2.65505, 1.3685, 1.79396, 2.96189, 1.45944,
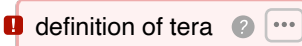 2.00506, 2.11244, 2.04871, 2.11311, 2.14469, 1.3798, 1.36292, 2.73289}

In[23]:=

In[24]:= `mus = UnitConvert[#, "Kilograms"] & /@ { 7.9995 u , 6.8605 u , 7.4684 u }`

Out[24]=

$\{ 1.32835 \times 10^{-26}$ kg , 1.13921×10^{-26} kg , 1.24016×10^{-26} kg $\}$

In[32]:= `nus =` $\sqrt{\dfrac{\#1}{\#2}} \dfrac{1}{2\pi}$ `&@@@ Transpose[{ks, mus}]` $\Big/$ `10^12 // Round[#, 0.1] &`

Out[32]=

$\{ 44.9$ per second , 57.5 per second , 52.3 per second $\}$

In[26]:= `100` $\dfrac{\#1 - \#2}{\#2}$ `&@@@ Transpose[{{47.4, 65.1, 59.3}, nus}] // Round[#, 0.01] &`

Out[26]=

{5.57, 13.22, 13.38}

In[27]:=

In[28]:= `QuantityMagnitude@ 1 THz`

Out[28]=

1

In[29]:= ⚠ definition of tera ❓ ⋯

Out[29]=

Failure[⚠

Message:	No Wolfram Language translation found.
Tag:	NoParse
Query:	definition of tera

]

Bond order pt3

In[35]:= `{d1, corr, mol} =`
`  Import["/Users/giovannigravili/Downloads/dati.txt.txt", "Table"] // Transpose`

Out[35]=

{{0.121703, 0.182656, 0.130626, 0.125691, 0.1503, 0.13544},
 {-0.00170271, -0.0626556, -0.0106262, -0.00569094, -0.0302999, -0.0154405},
 {O2, Li2, F2, C2, Be2, B2}}

In[42]:= `dat = d1 - corr`

Out[42]=

{0.123405, 0.245311, 0.141252, 0.131382, 0.1806, 0.150881}

In[40]:= `{b, mol2} =`
`Import["/Users/giovannigravili/Downloads/bond.txt.txt", "Table"] // Transpose`

Out[40]=
`{{2, 1, 1, 2, 0, 1}, {O2, Li2, F2, C2, Be2, B2}}`

In[41]:= `mol == mol2`

Out[41]=
`True`

In[57]:= `mol = {"O₂", "Li₂", "F₂", "C₂", "Be₂", "B₂"}`
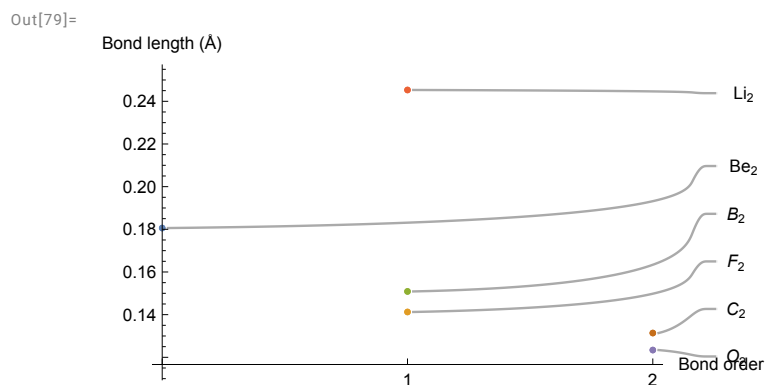
Out[57]=
$\{O_2, Li_2, F_2, C_2, Be_2, B_2\}$

In[59]:= `g = SortBy[Transpose[{b, dat, mol}], First]`

Out[59]=
$\{\{0, 0.1806, Be_2\}, \{1, 0.141252, F_2\}, \{1, 0.150881, B_2\},$
$\{1, 0.245311, Li_2\}, \{2, 0.123405, O_2\}, \{2, 0.131382, C_2\}\}$

In[61]:= `lbl = #3 & @@@ g`

Out[61]=
$\{Be_2, F_2, B_2, Li_2, O_2, C_2\}$

In[79]:= `plsst = ListPlot[SortBy[Transpose[{b, dat}], First] // Partition[#, 1] &,`
`PlotLabels → lbl, ImageSize → Medium, AxesLabel →`
`{"Bond order", "Bond length (Å)"}, Ticks → {Range[0, 2, 1], Automatic}]`

Out[79]=

In[80]:= `Export[`
`"/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM MANO/`
`Computational material physics /Lab reports/2/boplt.pdf", plsst]`

Out[80]=
`/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM`
`MANO/Computational material physics /Lab reports/2/boplt.pdf`