In[•]:=
```
Charting`$InteractiveHighlighting = False
```
Out[•]=
```
False
```

Part 2 molecules

In[•]:=
```
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[•]:=
```
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}, {0.67 , 0.81, 0.014}}}];
```

In[•]:=
```
Range[1.08, 1.32, 0.024 ] // Length
```
Out[•]=
```
11
```

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

In[•]:=
```
fits = Fit[#, {1, x, x^2}, x] & /@
  (Take[#1, {#2, -1}] & @@@ Transpose[{data2, {5, 5, 5}}])
```
Out[•]=
$$\left\{42.1132 - 81.9884\, x + 33.048\, x^2,\ 45.9343 - 106.094\, x + 46.3396\, x^2,\ 577.941 - 1267.77\, x + 693.512\, x^2\right\}$$

In[•]:=
```
coeffs = Fit[#, {1, x, x^2}, x, "BestFitParameters"] & /@
    (Take[#1, {#2, -1}] & @@@ Transpose[{data2, {5, 5, 5}}]);
```

In[ ]:=
```
Show[Plot[#1[d], {d, #3[[1]], #3[[2]]}, ImageSize → Medium,
    Epilog → {Point[#] & /@ #2}, PlotRange → All], Plot[#4, {x, #3[[1]], #3[[2]]},
    PlotStyle → {Orange, Dashed}, PlotRange → All, PlotLabel → #5]] & @@@ Transpose[
 {ip, data2, {{1.08, 1.35}, {1.02, 1.24}, {0.67, 0.81}}, fits, {"O2", "CO", "NO"}}]
```

Out[ ]=