```
> restart;
> l1:=[[0,-448.191911],[1,-443.160],[2,-438.272],[3,-433.44,triangle],[4,-428.557,tetra],[5,
  -423.795,octa]];
  E_Cu:=-200.863509;
```

$$l1 := [[0, -448.191911], [1, -443.160], [2, -438.272], [3, -433.44, triangle], [4, -428.557, tetra], [5, -423.795, octa]] \quad (1)$$

$$E\_Cu := -200.863509$$

```
> l2:=[];
  for i from 2 to nops(l1) do
  tmp:=l1[i][2]-(l1[1][2]/54*(54-l1[i][1])+E_Cu/54*l1[i][1]);
  l2:=[op(l2),[l1[i][1],tmp]];
  od:
```

$$l2 := [\,] \quad (2)$$

```
> l_1:=[[0,-1062.821673],[6,-1033.600583],[7,-1028.800277],[8,-1023.964417],[9,
  -1019.181350],[10,-1014.649054],[11,-1009.584060],[12,-1004.806817],[13,-1000.049106],
  [14,-995.610967],[15,-991.090844]];
  E_Cu2:=-475.564689;
```

$$l\_1 := [[0, -1062.821673], [6, -1033.600583], [7, -1028.800277], [8, -1023.964417], [9, -1019.181350], [10, -1014.649054], [11, -1009.584060], [12, -1004.806817], [13, -1000.049106], [14, -995.610967], [15, -991.090844]] \quad (3)$$

$$E\_Cu2 := -475.564689$$

```
> l_2:=[];
  for i from 2 to nops(l_1) do
  tmp:=l_1[i][2]-(l_1[1][2]/128*(128-l_1[i][1])+E_Cu2/128*l_1[i][1]);
  l_2:=[op(l_2),[l_1[i][1],tmp]];
  od:
```

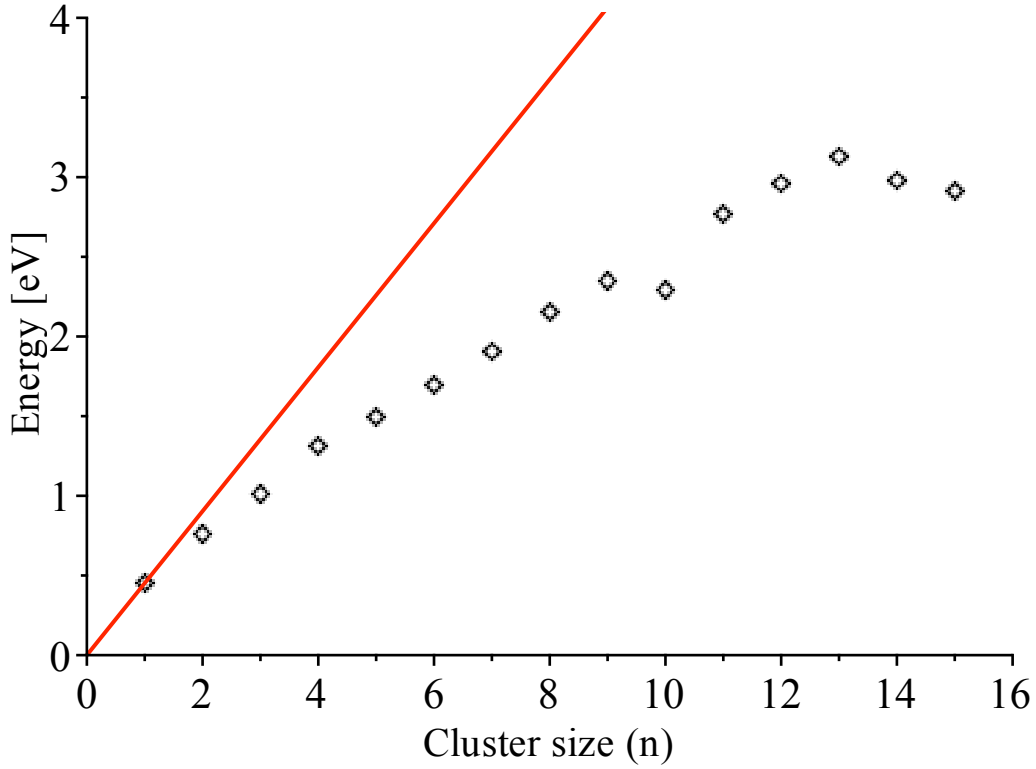
$$l\_2 := [\,] \quad (4)$$

```
> l_3:=[op(l2),op(l_2)];
  #128[1,0.46072781];
```

$$l\_3 := [[1, 0.451755411], [2, 0.759599822], [3, 1.01144423], [4, 1.31428864], [5, 1.49613306], [6, 1.69341880], [7, 1.90577893], [8, 2.15369486], [9, 2.34881640], [10, 2.29316703], [11, 2.77021566], [12, 2.95951399], [13, 3.12927963], [14, 2.97947316], [15, 2.91165079]] \quad (5)$$

```
> with(plots):
  with(stats):
Warning, the name changecoords has been redefined

> p1:=pointplot(l_3,symbolsize=15,view=[0..16,0..4],
  labels=["Cluster size (n)","Energy [eV]"],
  labeldirections=[horizontal,vertical],labelfont=[TIMES,ROMAN,14]):
> p2:=plot(l2[1][2]*n,n=0..16):
> display(p1,p2);
```




```
> l3:=[];
  for i from 2 to nops(l_3) do
  tmp:=l_3[i][2]-l_3[1][2]*l_3[i][1];
  l3:=[op(l3),[l_3[i][1],tmp]];
  od:
  l3;
```

$$l3 := [\,]$$ **(6)**

$$[[2, -0.143911000], [3, -0.343822003], [4, -0.492733004], [5, -0.762643995], [6, -1.017113666], [7, -1.256508947], [8, -1.460348428], [9, -1.716982299], [10, -2.224387080], [11, -2.199093861], [12, -2.461550942], [13, -2.743540713], [14, -3.345102594], [15, -3.864680375]]$$

```
> p3:=pointplot(l3,symbolsize=15,symbol=circle,
  labels=["Cluster size (n)","Energy [eV]"],
  labeldirections=[horizontal,vertical],labelfont=[TIMES,ROMAN,14]):
> l3_data1:=[];
  l3_data2:=[];
  for i from 1 to nops(l3) do
  l3_data1:=[op(l3_data1),l3[i][1]];
  l3_data2:=[op(l3_data2),l3[i][2]];
  od:
  l3_data:=[l3_data1,l3_data2]:
```

$$l3\_data1 := [\,]$$ **(7)**

$$l3\_data2 := [\,]$$

```
> c:=-0.41:
  f1:=n->c*(n-n^(2/3)):
  #fit1:=fit[leastsquare[[n,y], y=c*(n-n^(2/3)), {c}]](l3_data):
```

```
#f1:=unapply(rhs(fit1),n);
p4:=plot(f1(n),n=0..30,y=-1..0):
```

```
> c0:=0.014:
k:=0.8617*10^(-4);
T:=273+550;
p5:=plot(-k*T*(n-1)*ln(c0),n=1..30,color=blue):
p6:=plot(f1(n)-k*T*(n-1)*ln(c0),n=1..30):
```

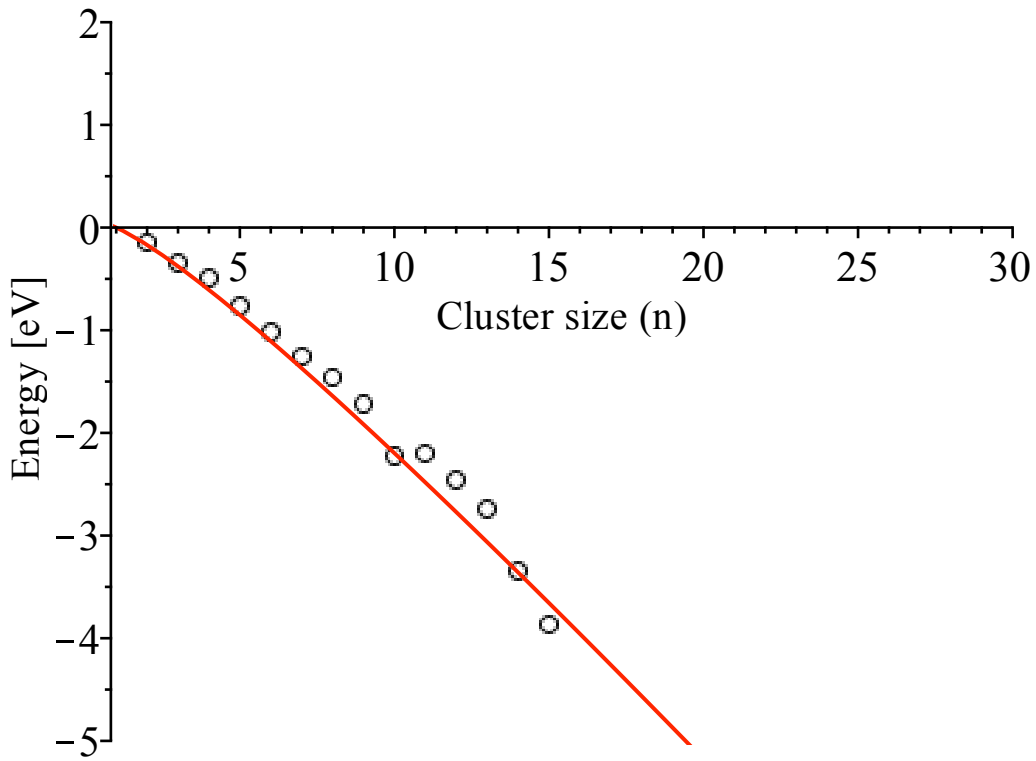
$$k := 0.00008617000000 \quad \textbf{(8)}$$

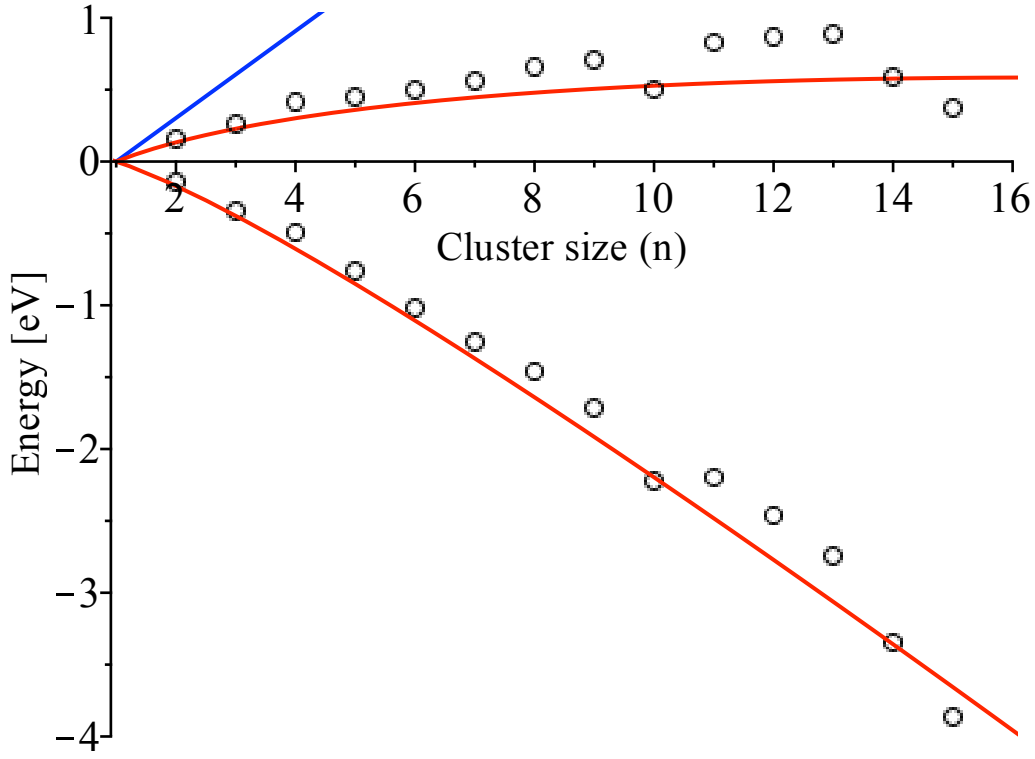
$$T := 823$$

```
> l3;
l4:=[]:
for i from 1 to nops(l3) do
l4:=[op(l4),[l3[i][1],l3[i][2]-k*T*(l3[i][1]-1)*ln(c0)]];
od:
p7:=pointplot(l4,symbolsize=15,symbol=circle):
```

$$[[2, -0.143911000], [3, -0.343822003], [4, -0.492733004], [5, -0.762643995], [6, -1.017113666], [7, -1.256508947], [8, -1.460348428], [9, -1.716982299], [10, -2.224387080], [11, -2.199093861], [12, -2.461550942], [13, -2.743540713], [14, -3.345102594], [15, -3.864680375]] \quad \textbf{(9)}$$

```
> display(p3,p4,view=[1..30,-5..2]);
display(p3,p4,p5,p6,p7,view=[1..16,-4..1]);
```






```
> solset:=solve(n-n^(2/3)=1,n):
  c_prime:=-evalf(f1(solset));
```

$$c\_prime := 0.4099999996 \quad \textbf{(10)}$$

```
> a:=2.867*10^(-10):
  V:=(a^3)/2:
  eq1:=(3*V)^(2/3)*(4*Pi)^(1/3)*sigma=c_prime*1.60219*10^(-19):
  sig:=evalf(solve(eq1,sigma));
```

$$sig := 0.2623282285 \quad \textbf{(11)}$$

```
> G:=n->f1(n)-k*T*(n-1)*ln(c0);
```

$$G := n \rightarrow f1(n) - k\,T\,(n-1)\ln(c0) \quad \textbf{(12)}$$

```
> DG:=diff(G(n),n):
  DG:=unapply(DG,n):
> CR:=solve(DG(n)=0,n);
  activity_energy:=evalf(G(CR));
```

$$CR := 16.54276795 \quad \textbf{(13)}$$

$$activity\_energy := 0.584567904$$