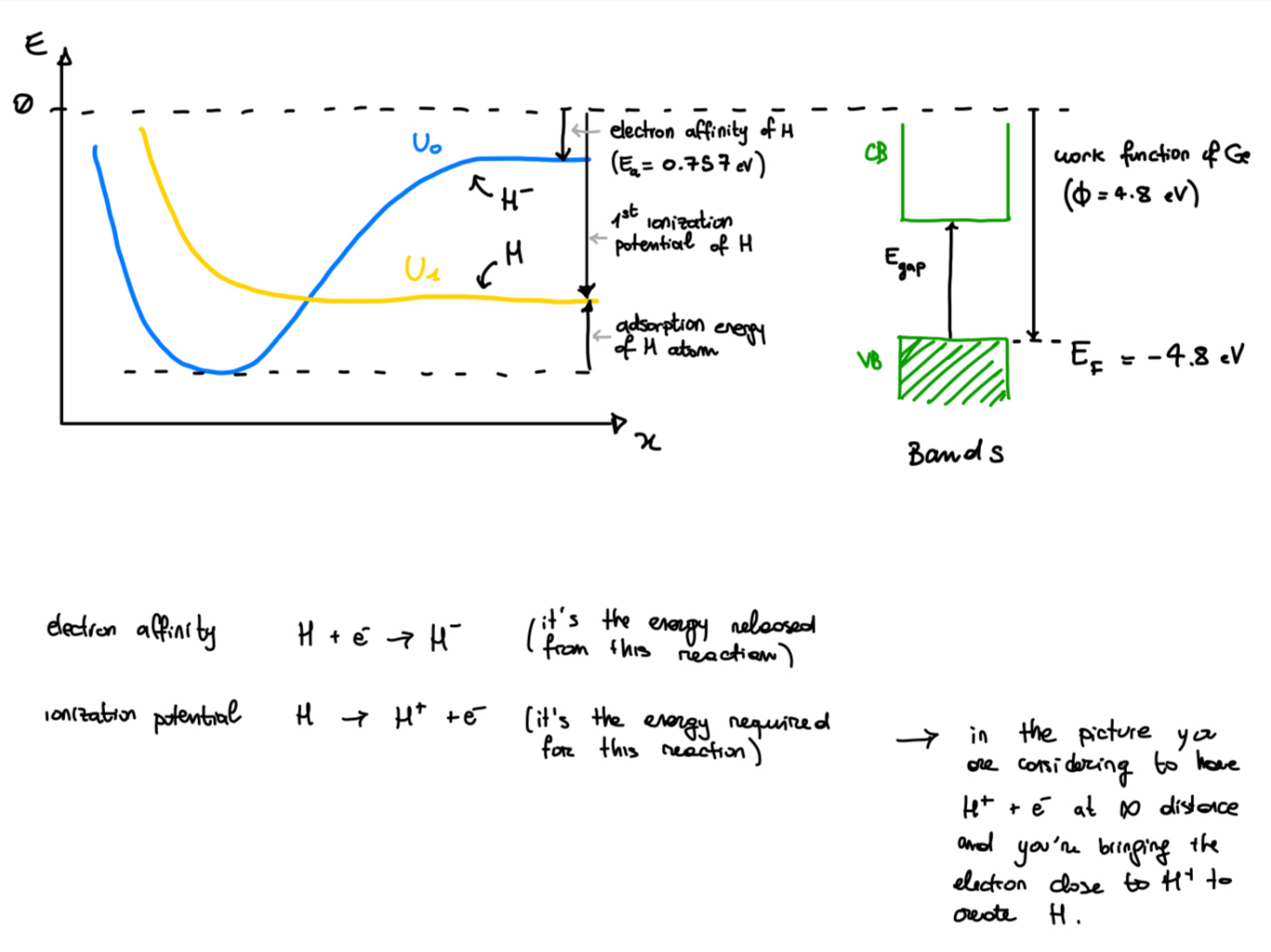
Design of $h(x)$

Why does Hokseon work on this?

On Friday 31st May 2024, Reini and Hokseon decided to shift our attention back to the H/H^- scattering on **Germanium** 锗 from H/H^+. In this sense, the impurity state $h(x) = U_1 - U_0$ will begin in the conduction band when $x = 5$Å. It goes down to the band gap and embrace into the valence band. The adiabatic PESs' gap would close when the impurity $h(x)$ hits the valence band. Because the valence band obtains an extra state but remains the same total number of electrons.

Images courtesy of **Sara Oregioni**, 2024.



Here above, we have some basic constraints for the $h(x)$ such as *electronic affinity* and *ionisation energy* of the H atom.

In the end, the adiabatic PES should look like

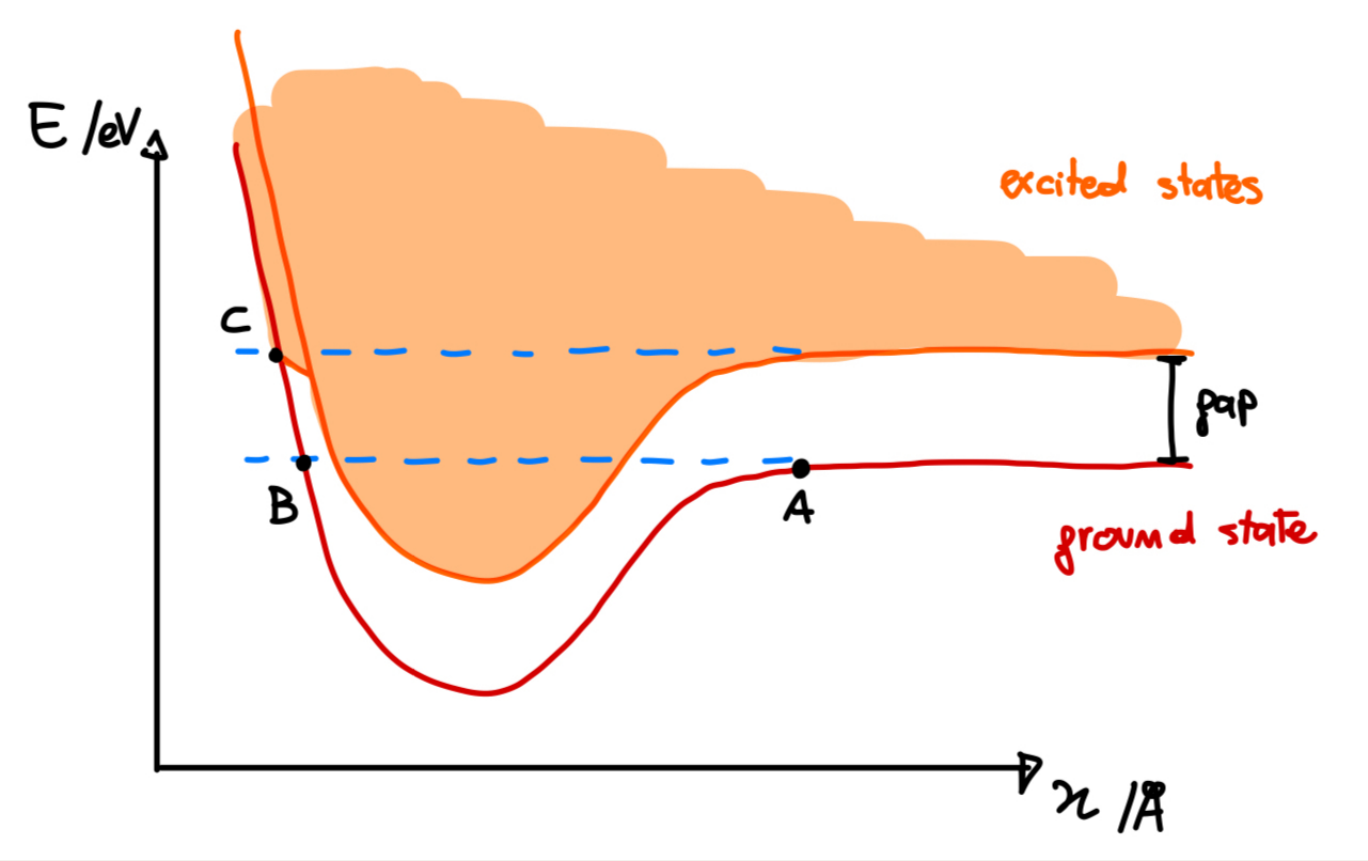
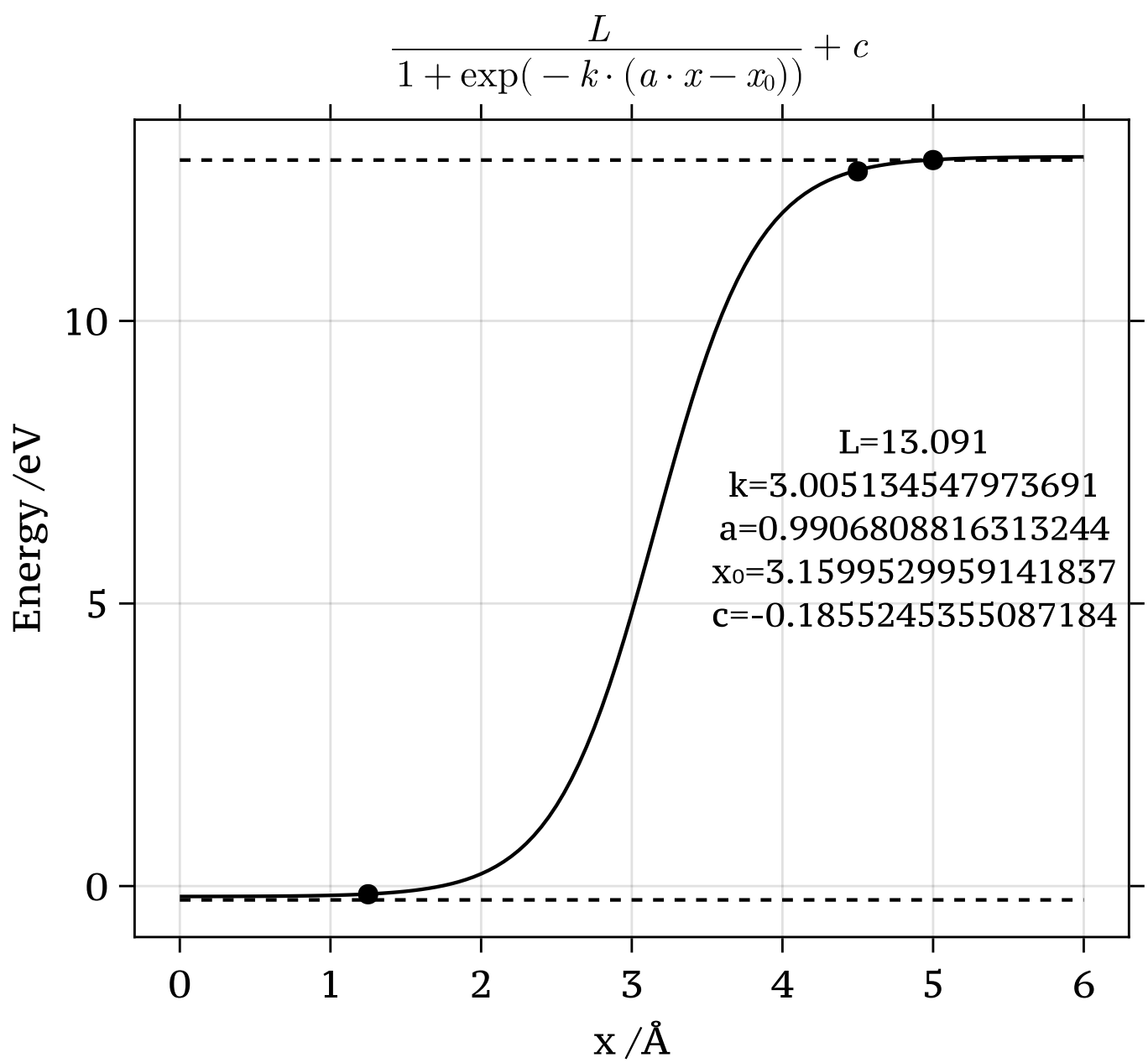


Image courtesy of **Sara Oregioni**, 2024

Sigmoid Functions

A **sigmoid function** is any mathematical function whose graph has a characteristic S-shaped or **sigmoid curve**.

Logistic Function



Black dots' coordinates

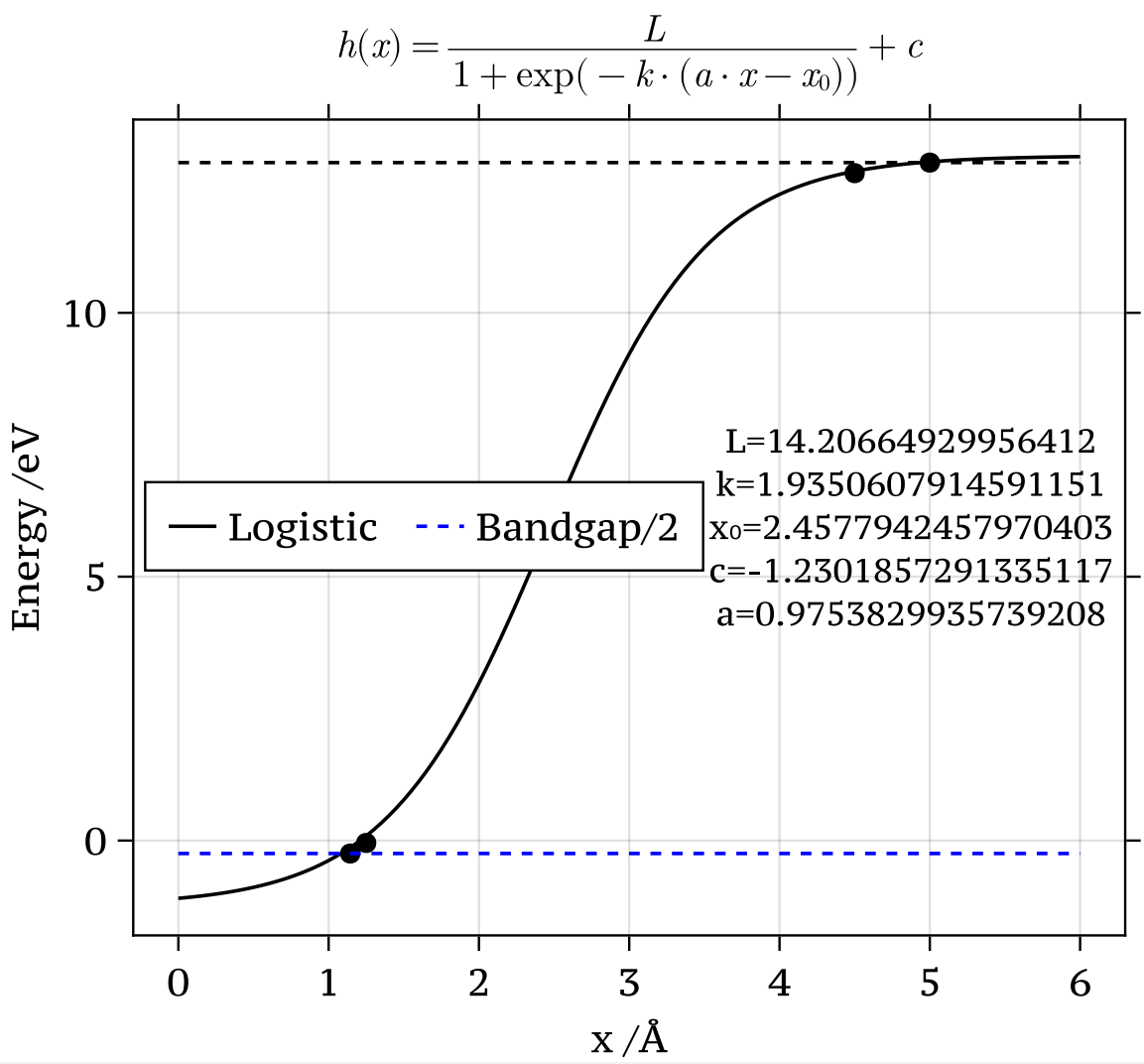
```
ϵ = 0.2
data_points = [(5,ionization_energy - electron_affinity),
               (4.5, ionization_energy - electron_affinity - ϵ),
               (1.25, -bandgap/2 + ϵ)]
```

What to do next

- Integrate this sigmoid function into NQCModels.jl
- Use sigmoid in Hokseon model for plotting the Adiabatic PES

Weekly Results

Okay Logistic Function Fit for $h(x)$



The fitting data are given as

```
data_points = [(5,ionization_energy - electron_affinity),
               (4.5, ionization_energy - electron_affinity - ϵ),
               (1.25, -bandgap/2 + ϵ),
               (1.144, -bandgap/2)]
```

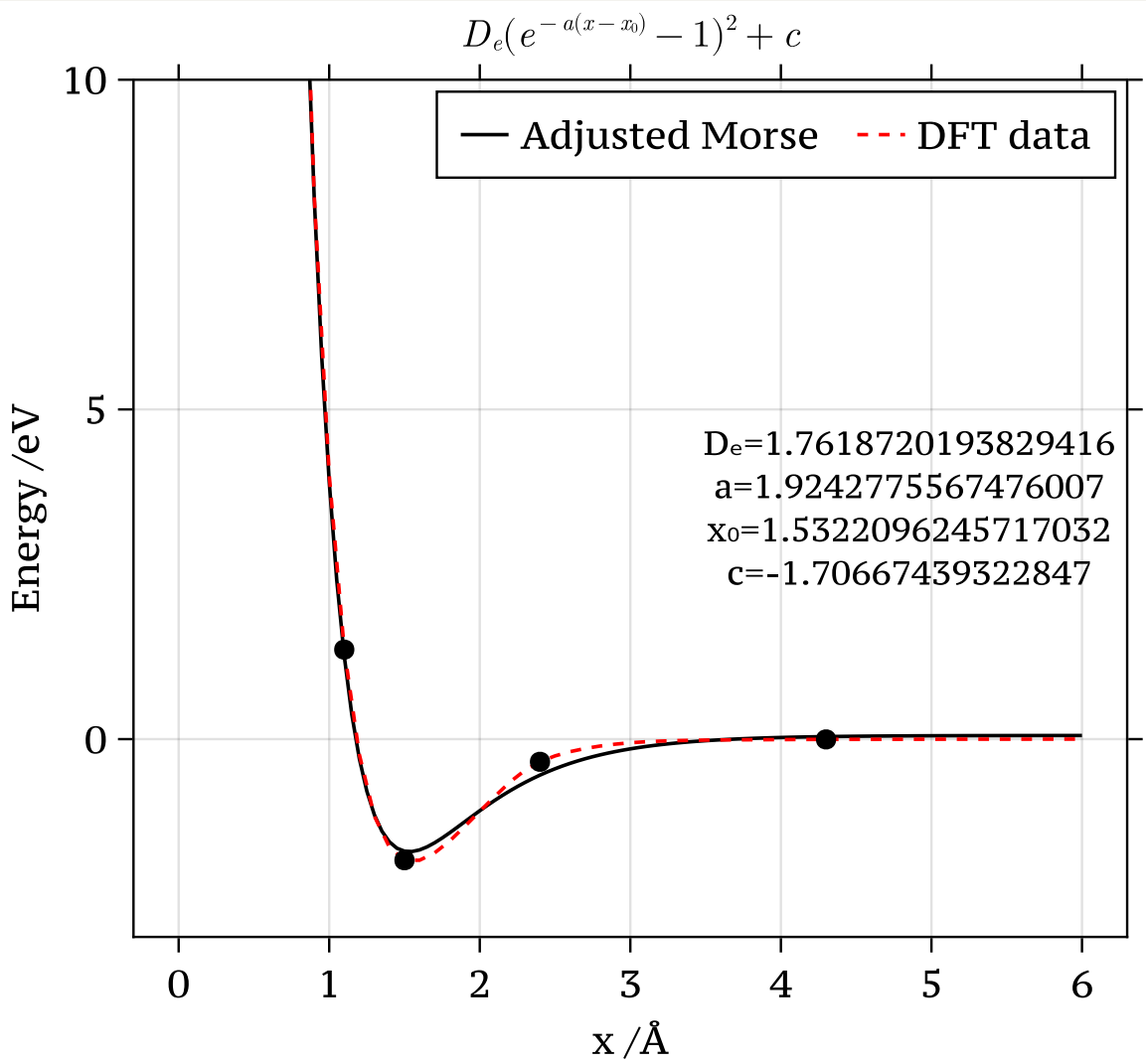
The upper dashed line stands for the energy:

$$\text{ionization energy} - \text{electron affinity} = 13.6\text{eV} - 0.754\text{eV}$$

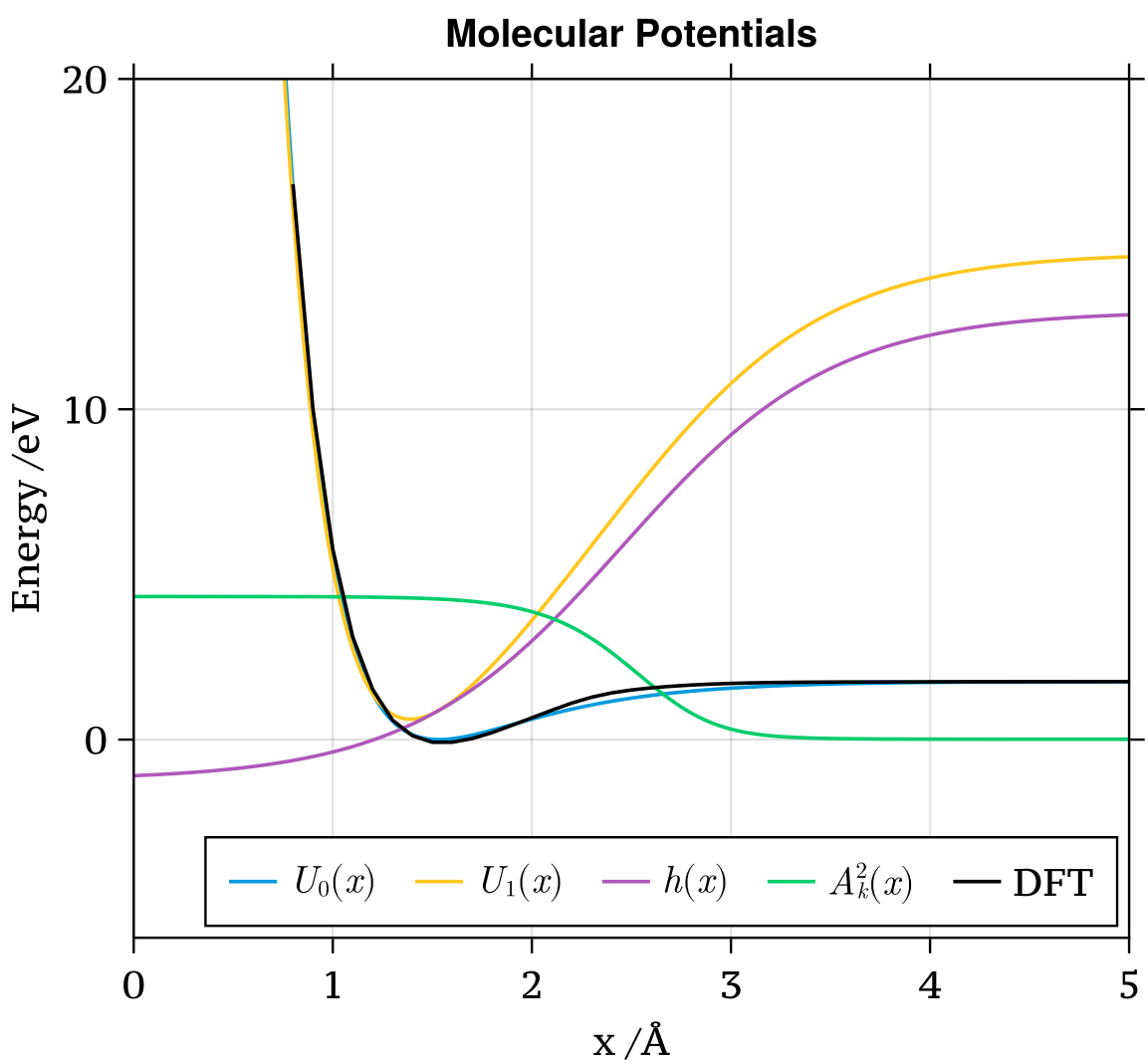
Alright Morse Potential Fit as U_0

It works when Γ_k is relatively small (adiabatic case?)

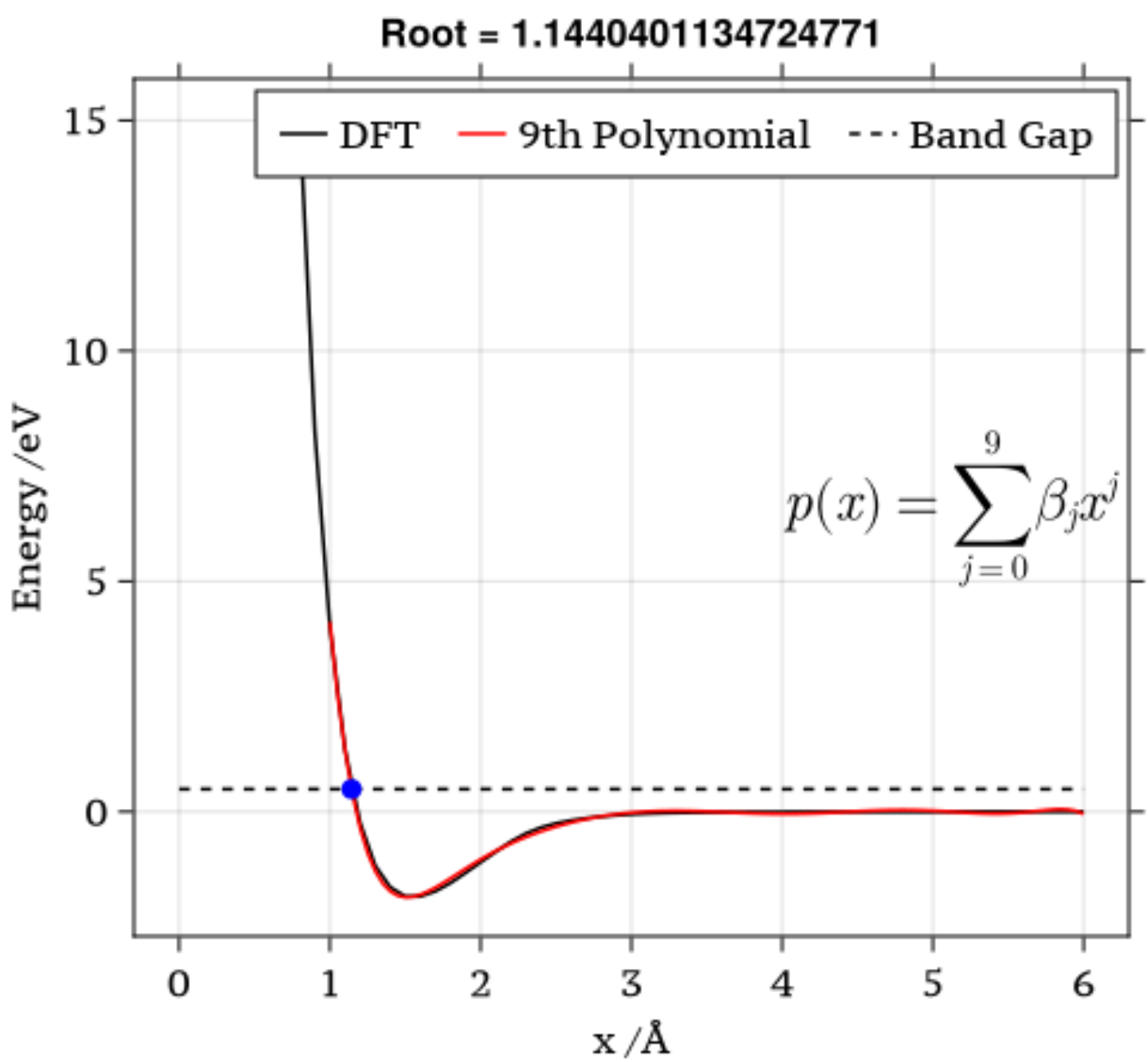
The morse potential is fitted from the DFT data of restatom.



Given $h(x)$ and U_0, we should have U_1, I call it Hokseon model



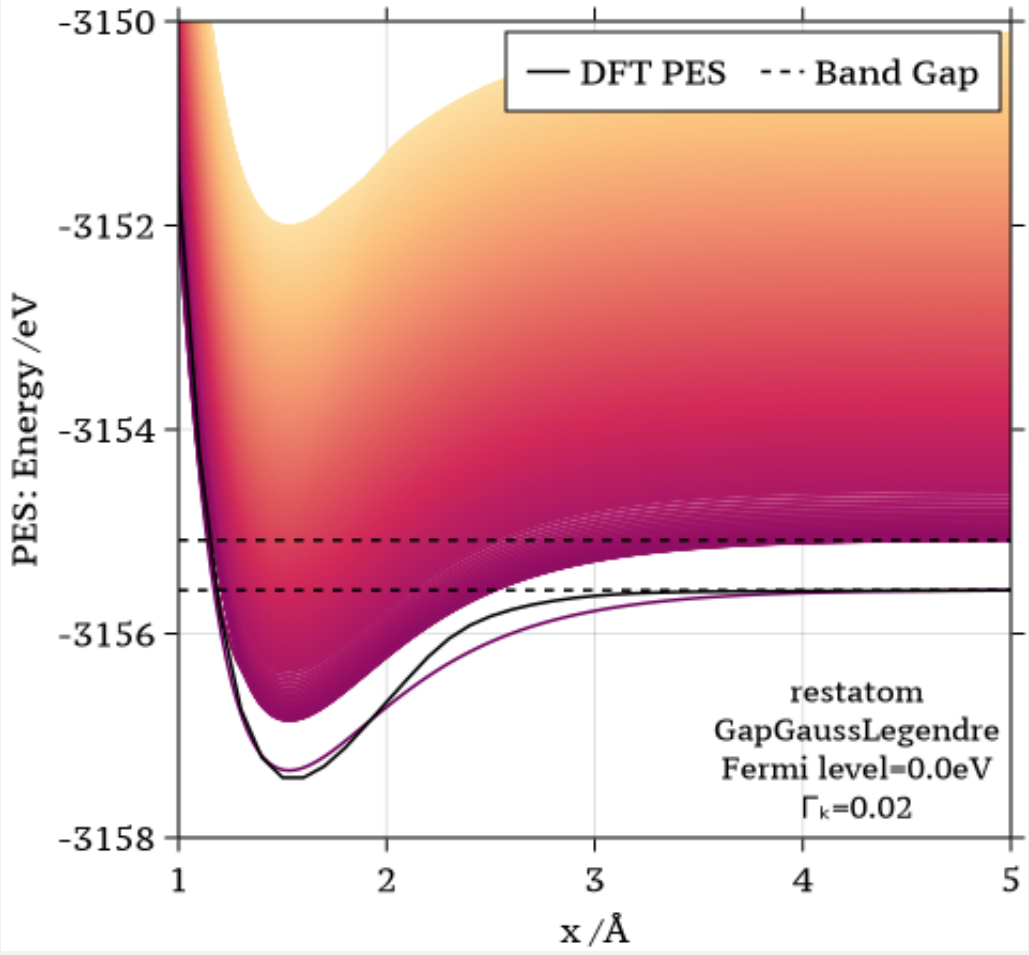
Location That The Gap Should Close

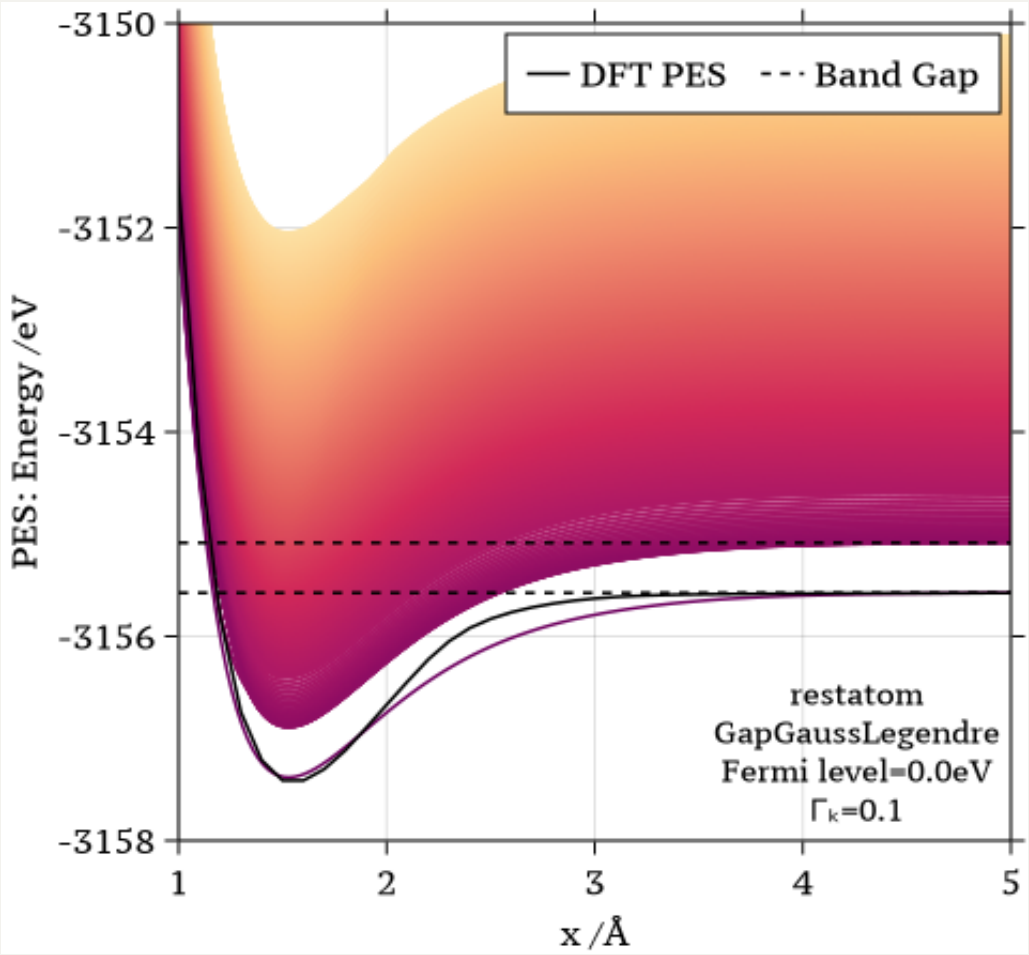


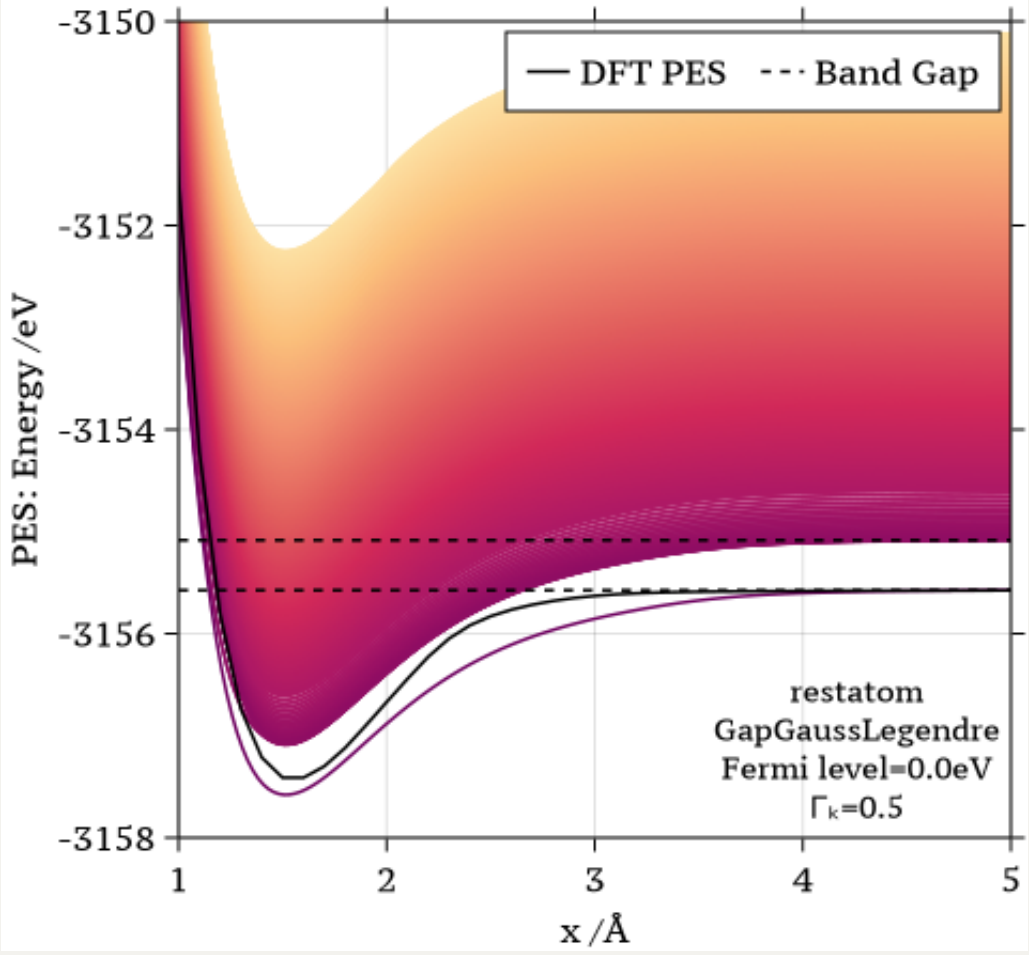
Basically, I fitted a polynomial and solve the solution at $\text{Energy} = 0.49\text{eV}$. So ideally, our adiabatic PESs should have a closing point at 1.144 Å.

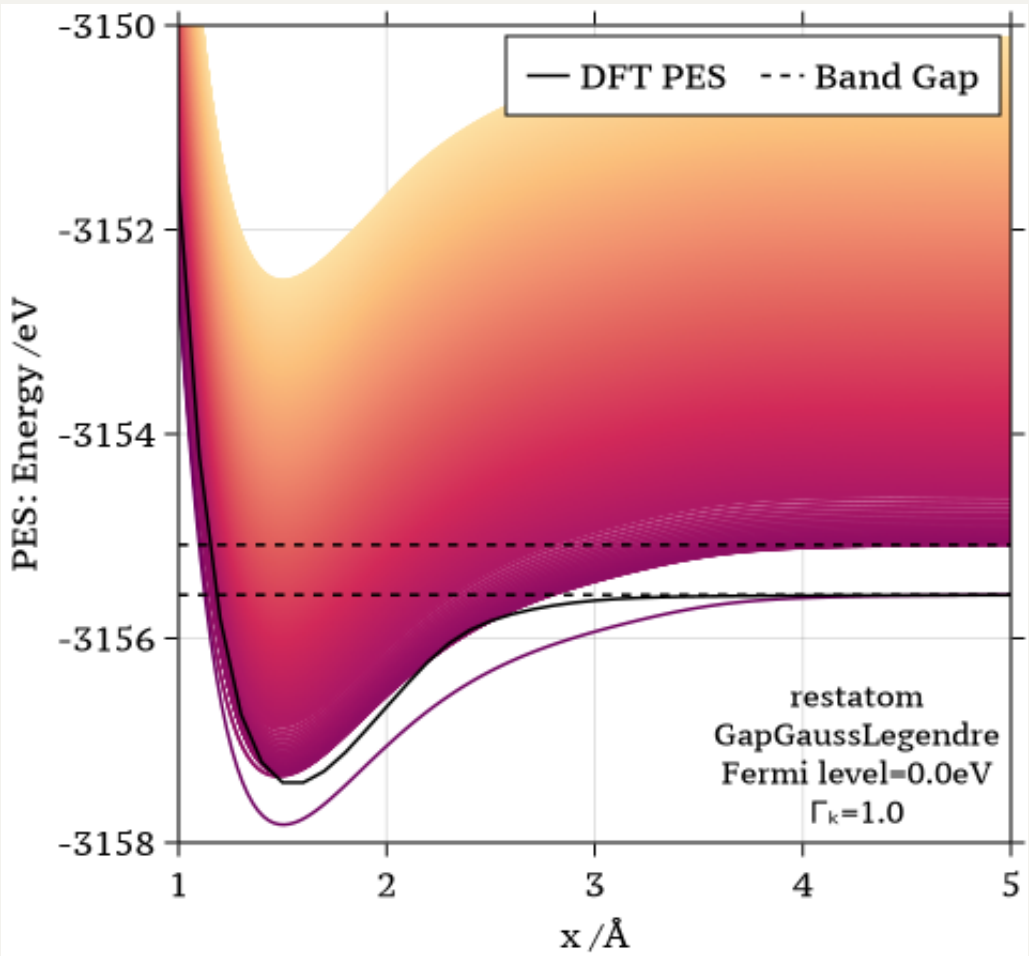
Alright Adiabatic PESs

Generally the hybridisation is weaker, the fitted parameters work better.


DFT PES
Band Gap
-3150
-3152
-3154
-3156
-3158
PES: Energy /eV
1
2
3
4
5
x /Å
restatom
GapGaussLegendre
Fermi level=0.0eV
Γk=0.02


DFT PES
Band Gap
-3150
-3152
-3154
-3156
-3158
PES: Energy /eV
1
2
3
4
5
x /Å
restatom
GapGaussLegendre
Fermi level=0.0eV
Γk=0.1


DFT PES
Band Gap
-3150
-3152
-3154
-3156
-3158
PES: Energy /eV
1
2
3
4
5
x /Å
restatom
GapGaussLegendre
Fermi level=0.0eV
Γk=0.5


DFT PES
Band Gap
-3150
-3152
-3154
-3156
-3158
PES: Energy /eV
1
2
3
4
5
x /Å
restatom
GapGaussLegendre
Fermi level=0.0eV
Γk=1.0

Zoom In Versions

$\Gamma_k = 0.02$

$\Gamma_k = 0.1$

$\Gamma_k = 0.5$

$\Gamma_k = 1.0$

Hokseon's Thoughts

- When we have noticeable hybridisation, we shouldn't rely on the parameters from the Least Square fitting. We probably need to tune the parameters manually.
- Still need to think about the crossing point problem. Because the gap closes later than 1.144 Å.