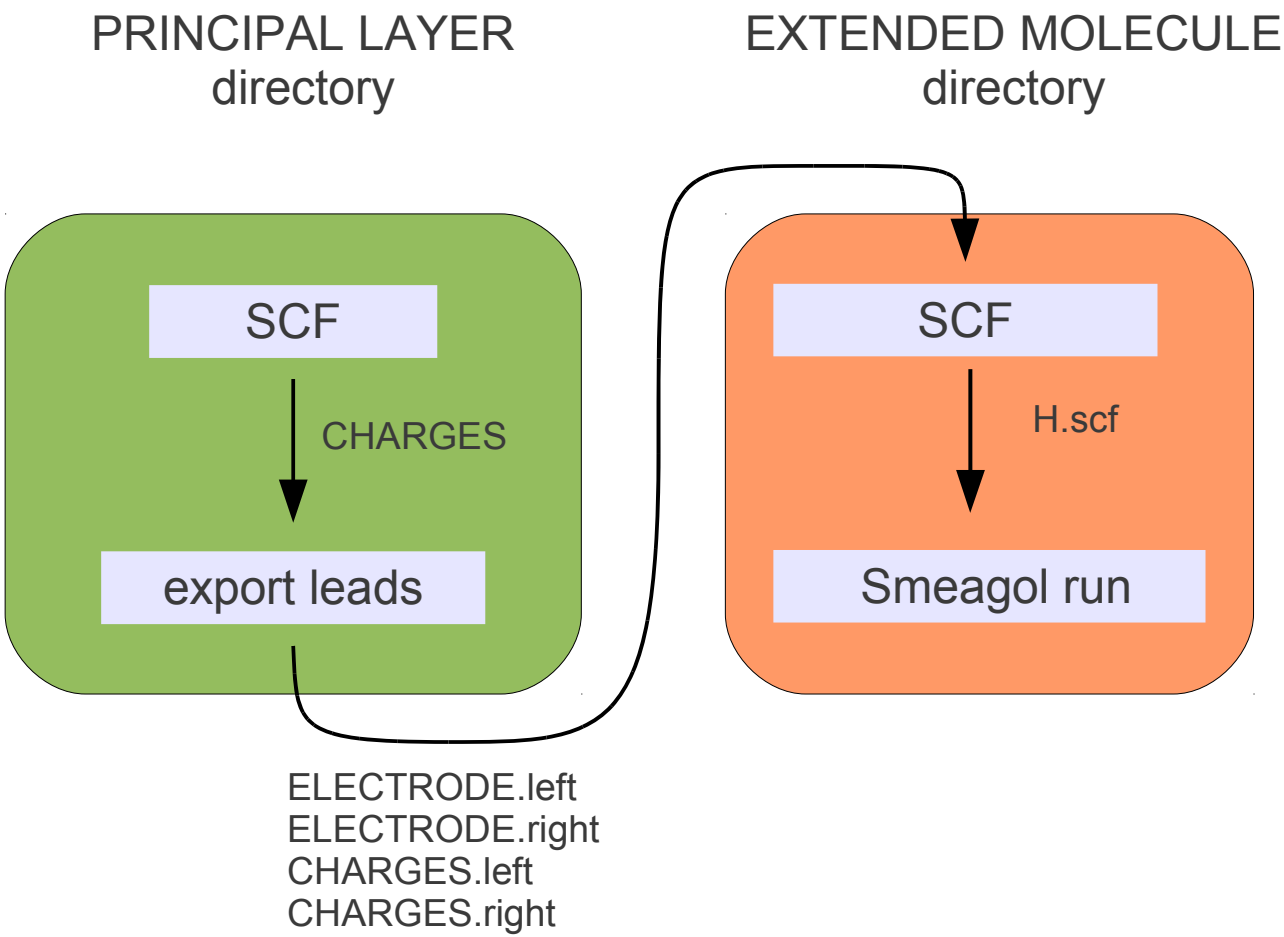
Basic scheme of Fireball2Smeagol Run



BULK calculation

answer.bas [----] 0 L:[1+ 0 1/ 7]

element 6	x	y	z
1	3.000000	3.000000	1.000000
1	3.000000	3.000000	2.000000
1	3.000000	3.000000	3.000000
1	3.000000	3.000000	4.000000
1	3.000000	3.000000	5.000000
1	3.000000	3.000000	6.000000

cel.lvs [----] 20 L:[1+ 2 3/ 4]

20.0000000000	0.0000000000	0.0000000000
0.0000000000	20.0000000000	0.0000000000
0.0000000000	0.0000000000	6.0000000000

fireball.in [----] 13 L

```
&OPTION
basisfile = answer.bas
lvsfile = cel.lvs
icluster = 0
nstepf = 1
sigmatol = 0.0000000001
max_scf_iterations = 100
dt = 0.5
iqout = 1
ismeagol = 0
ifixcharge = 0
&END

&OUTPUT
iwrtHSrho = 0
iwrteigen = 0
iwrtdos = 0
&END

&QUENCH
&END

&MESH
&END
```

SCF

fireball.in [----] 1

```
&OPTION
basisfile = answer.bas
lvsfile = cel.lvs
icluster = 0
nstepf = 1
sigmatol = 0.0000000001
max_scf_iterations = 100
dt = 0.5
iqout = 1
ismeagol = 0
ifixcharge = 1
&END

&OUTPUT
iwrtHSrho = 1
iwrteigen = 0
iwrtdos = 0
&END

&QUENCH
&END

&MESH
&END
```

export leads

input.kpts [----] 0 L:[1+ 0 1/102] *(0 /6956b)= 32

```
 100
 0.0000000000   0.0000000000    -0.5183627873          0.0100000000
 0.0000000000   0.0000000000    -0.5078908118          0.0100000000
 0.0000000000   0.0000000000    -0.4974188363          0.0100000000
 0.0000000000   0.0000000000    -0.4869468608          0.0100000000
 0.0000000000   0.0000000000    -0.4764748853          0.0100000000
```

k-points in x,y,z (for bulk)

MOLECULE.kpts [----] 0 L:[1+ 2 3/ 3] *(73 / 73b)= <EOF>

```
  1
 0.0000000000   0.0000000000    0.0000000000          1.0000000000
```

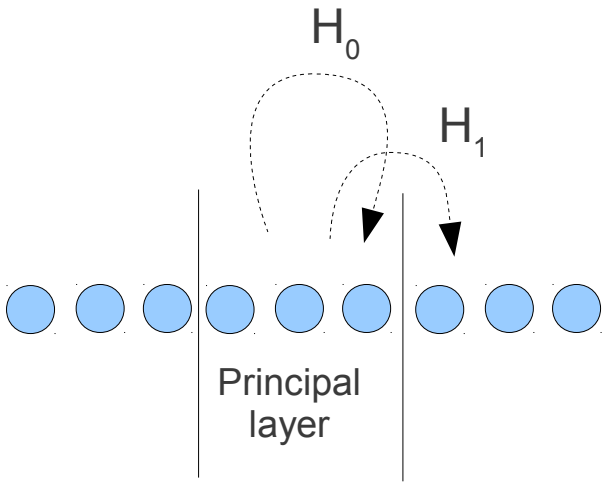
k-points in x,y (for exported leads)

Projection
H, S, ρ

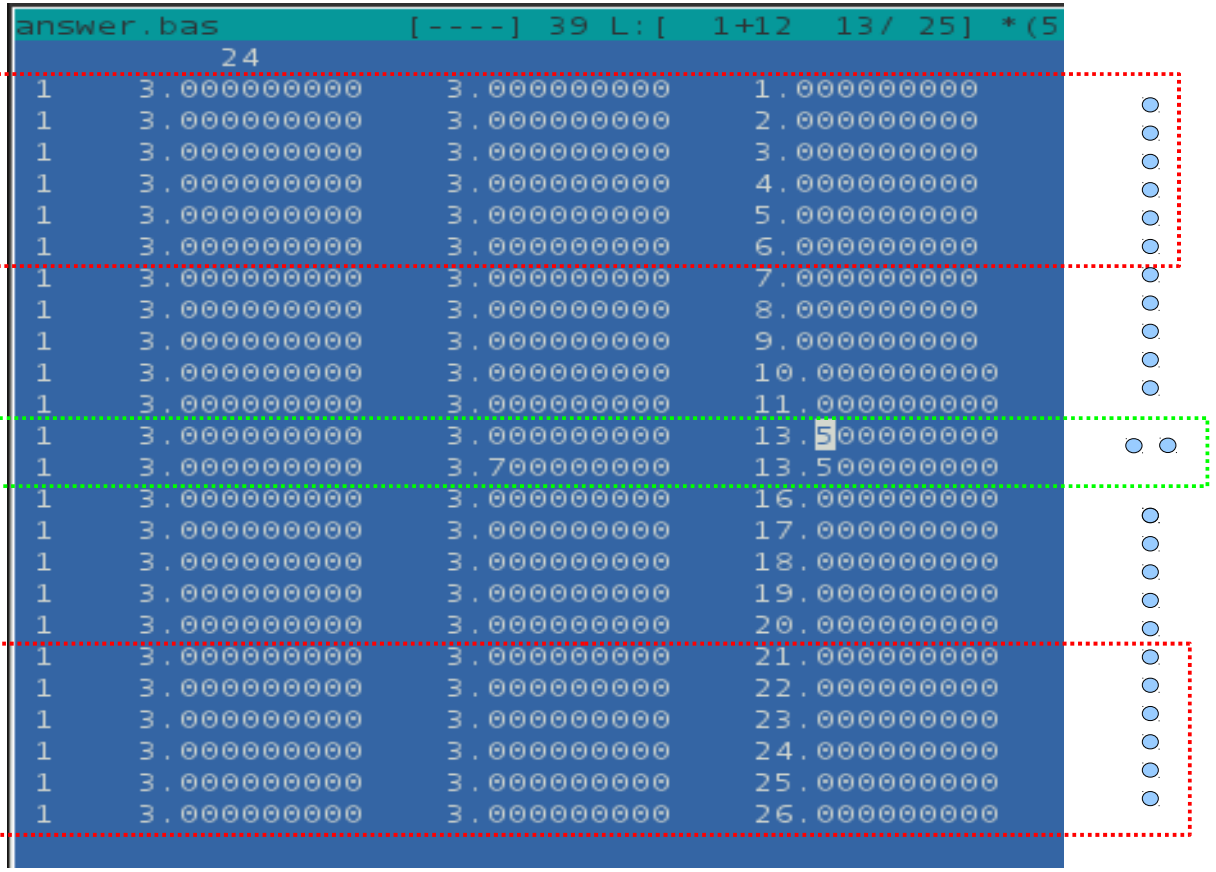
output to "ELECTRODE" file

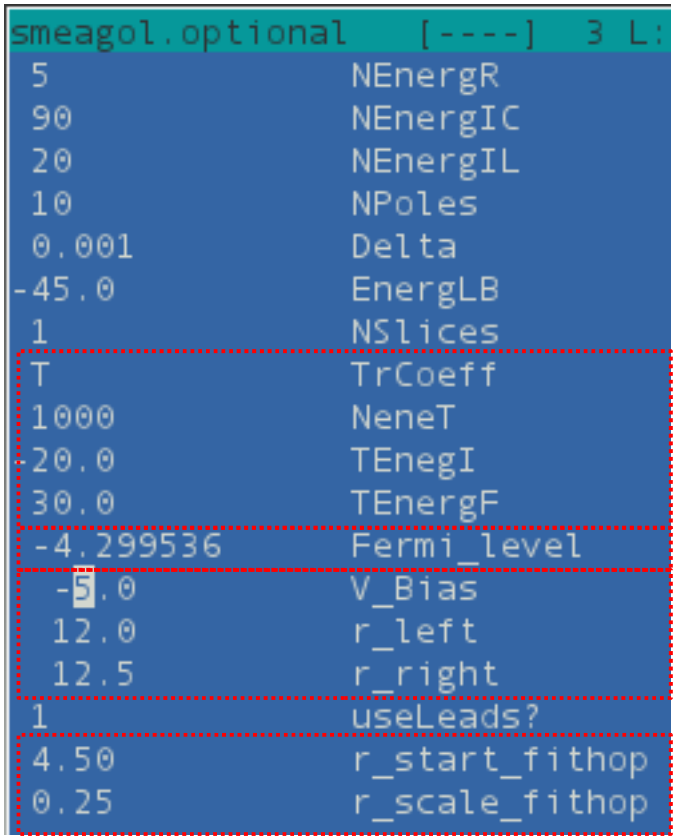
```
ELECTRODE.left      [----]  0 L:[  1+38  39/ 39] *(7040/7040b)= <EOF>
     6          100          1
     1  0.000000E+00  0.000000E+00  0.000000E+00
     1           1 -0.891501E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.100000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.651952E+00  0.000000E+00  0.000000E+00  0.000000E+00
     1           2 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00  0.000000E+00  0.000000E+00
     1           3 -0.302697E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.127210E+00  0.000000E+00  0.000000E+00  0.000000E+00 -0.162768E+00  0.000000E+00  0.000000E+00  0.000000E+00
     1           4 -0.423428E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.802623E-02  0.000000E+00  0.000000E+00  0.000000E+00 -0.221685E+00  0.000000E+00  0.000000E+00  0.000000E+00
     1           5 -0.643532E-02  0.000000E+00  0.000000E+00  0.000000E+00  0.700987E-05  0.000000E+00  0.000000E+00  0.000000E+00  0.625946E-01  0.000000E+00  0.000000E+00  0.000000E+00
     1           6  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
     2           1 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00  0.000000E+00  0.000000E+00
     2           2 -0.891501E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.100000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.651952E+00  0.000000E+00  0.000000E+00  0.000000E+00
     2           3 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00  0.000000E+00  0.000000E+00
     2           4 -0.302697E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.127210E+00  0.000000E+00  0.000000E+00  0.000000E+00 -0.162768E+00  0.000000E+00  0.000000E+00  0.000000E+00
     2           5 -0.423428E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.802623E-02  0.000000E+00  0.000000E+00  0.000000E+00 -0.221685E+00  0.000000E+00  0.000000E+00  0.000000E+00
     2           6 -0.643532E-02  0.000000E+00  0.000000E+00  0.000000E+00  0.700987E-05  0.000000E+00  0.000000E+00  0.000000E+00  0.625946E-01  0.000000E+00  0.000000E+00  0.000000E+00
     3           1 -0.302697E+01  0.000000E+00 -0.643532E-02  0.000000E+00  0.127210E+00  0.000000E+00  0.700987E-05  0.000000E+00 -0.162768E+00  0.000000E+00  0.625946E-01  0.000000E+00
     3           2 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00  0.000000E+00  0.000000E+00
     3           3 -0.891501E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.100000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.651952E+00  0.000000E+00  0.000000E+00  0.000000E+00
     3           4 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00  0.000000E+00  0.000000E+00
     3           5 -0.302697E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.127210E+00  0.000000E+00  0.000000E+00  0.000000E+00 -0.162768E+00  0.000000E+00  0.000000E+00  0.000000E+00
     3           6 -0.423428E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.802623E-02  0.000000E+00  0.000000E+00  0.000000E+00 -0.221685E+00  0.000000E+00  0.000000E+00  0.000000E+00
     4           1 -0.423428E+00  0.000000E+00 -0.423428E+00  0.000000E+00  0.802623E-02  0.000000E+00  0.802623E-02  0.000000E+00 -0.221685E+00  0.000000E+00 -0.221685E+00  0.000000E+00
     4           2 -0.302697E+01  0.000000E+00 -0.643532E-02  0.000000E+00  0.127210E+00  0.000000E+00  0.700987E-05  0.000000E+00 -0.162768E+00  0.000000E+00  0.625946E-01  0.000000E+00
     4           3 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00  0.000000E+00  0.000000E+00
     4           4 -0.891501E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.100000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.651952E+00  0.000000E+00  0.000000E+00  0.000000E+00
     4           5 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00  0.000000E+00  0.000000E+00
     4           6 -0.302697E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.127210E+00  0.000000E+00  0.000000E+00  0.000000E+00 -0.162768E+00  0.000000E+00  0.000000E+00  0.000000E+00
     5           1 -0.643532E-02  0.000000E+00 -0.302697E+01  0.000000E+00  0.700987E-05  0.000000E+00  0.127210E+00  0.000000E+00  0.625946E-01  0.000000E+00 -0.162768E+00  0.000000E+00
     5           2 -0.423428E+00  0.000000E+00 -0.423428E+00  0.000000E+00  0.802623E-02  0.000000E+00  0.802623E-02  0.000000E+00 -0.221685E+00  0.000000E+00 -0.221685E+00  0.000000E+00
     5           3 -0.302697E+01  0.000000E+00 -0.643532E-02  0.000000E+00  0.127210E+00  0.000000E+00  0.700987E-05  0.000000E+00 -0.162768E+00  0.000000E+00  0.625946E-01  0.000000E+00
     5           4 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00  0.000000E+00  0.000000E+00
     5           5 -0.891501E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.100000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.651952E+00  0.000000E+00  0.000000E+00  0.000000E+00
     5           6 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00  0.000000E+00  0.000000E+00
     6           1  0.000000E+00  0.000000E+00 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00
     6           2 -0.643532E-02  0.000000E+00 -0.302697E+01  0.000000E+00  0.700987E-05  0.000000E+00  0.127210E+00  0.000000E+00  0.625946E-01  0.000000E+00 -0.162768E+00  0.000000E+00
     6           3 -0.423428E+00  0.000000E+00 -0.423428E+00  0.000000E+00  0.802623E-02  0.000000E+00  0.802623E-02  0.000000E+00 -0.221685E+00  0.000000E+00 -0.221685E+00  0.000000E+00
     6           4 -0.302697E+01  0.000000E+00 -0.643532E-02  0.000000E+00  0.127210E+00  0.000000E+00  0.700987E-05  0.000000E+00 -0.162768E+00  0.000000E+00  0.625946E-01  0.000000E+00
     6           5 -0.819445E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.580044E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.338783E+00  0.000000E+00  0.000000E+00  0.000000E+00
     6           6 -0.891501E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.100000E+01  0.000000E+00  0.000000E+00  0.000000E+00  0.651952E+00  0.000000E+00  0.000000E+00  0.000000E+00
μ        ν   Re H0        Im H0        Re H1        Im H1        Re S0        Im S0        Re S1        Im S1        Re ρ0        Im ρ0        Re ρ1        Im ρ1
```

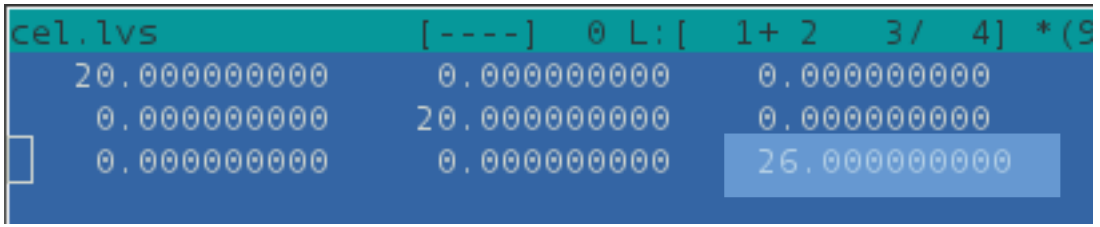
$$
\begin{pmatrix}
0 & H_{-1} & H_0 & H_1 & 0 & . & . & . & . \\
. & 0 & H_{-1} & H_0 & H_{LM} & 0 & . & . & . \\
. & . & 0 & H_{ML} & H_M & H_{MR} & 0 & . & . \\
. & . & . & 0 & H_{RM} & H_0 & H_1 & 0 & . \\
. & . & . & . & 0 & H_{-1} & H_0 & H_1 & 0
\end{pmatrix}
$$

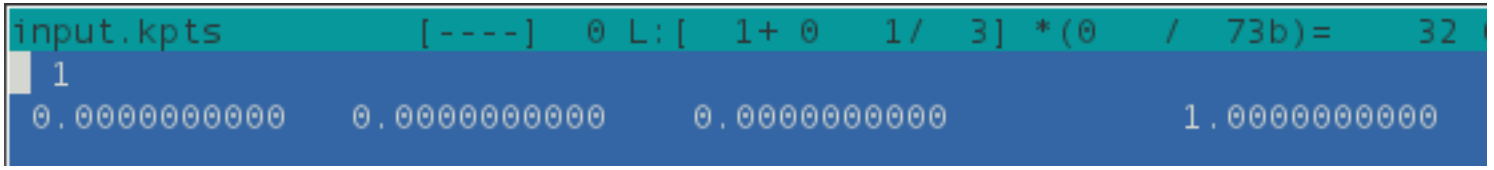


Extended molecule calculation



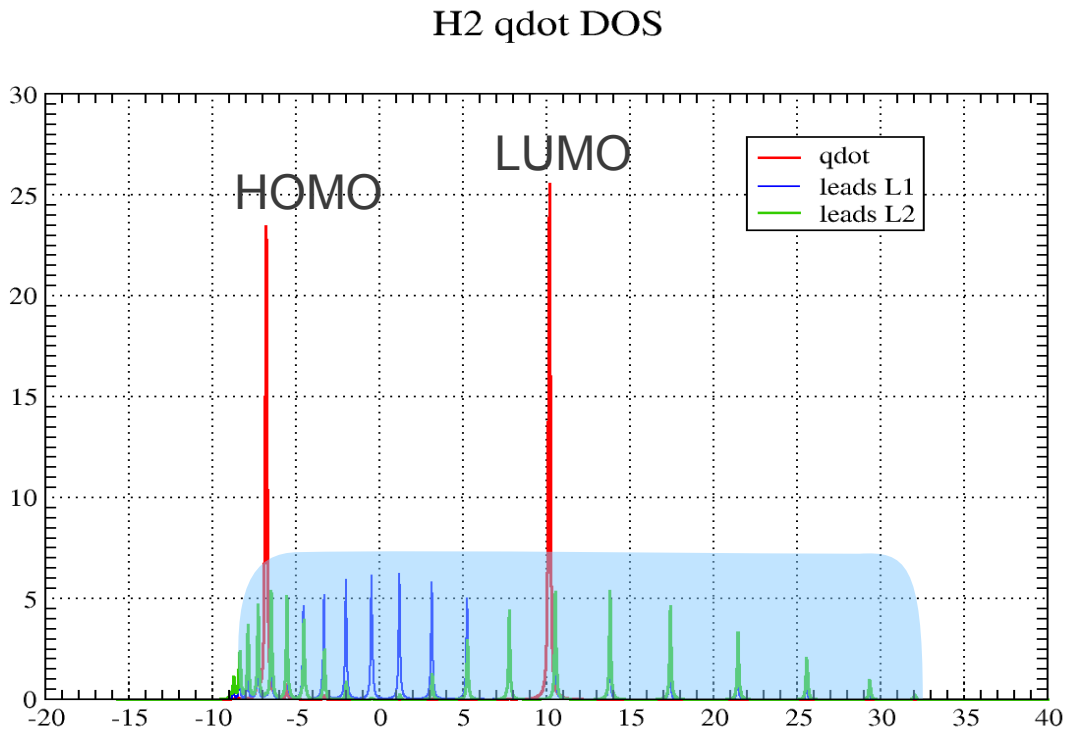


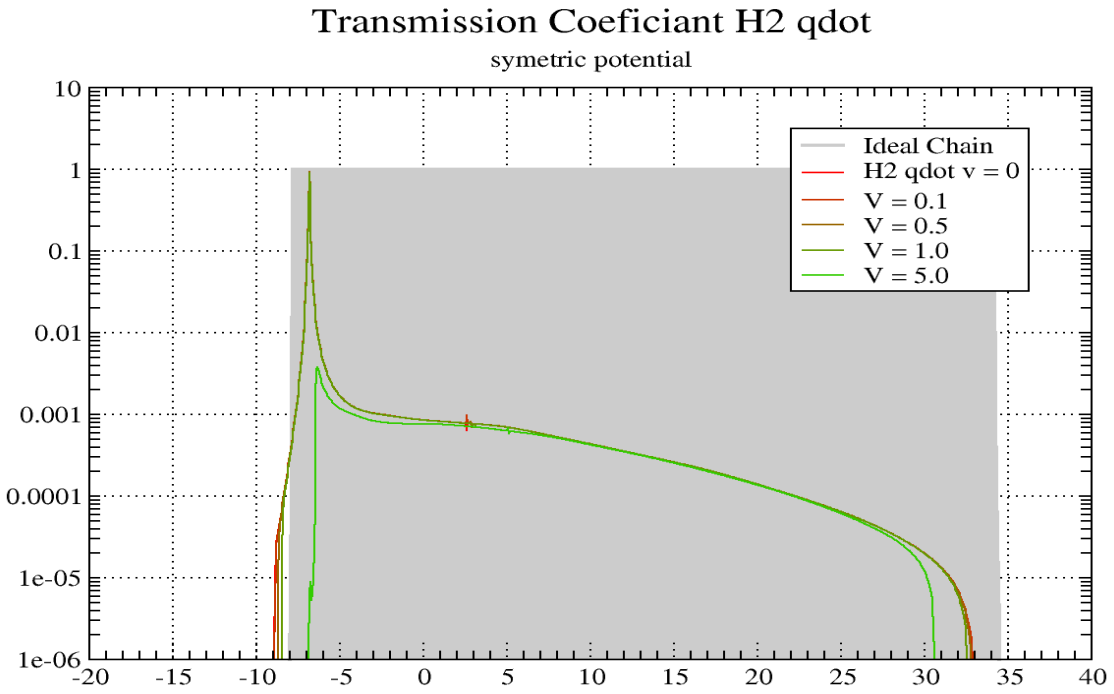


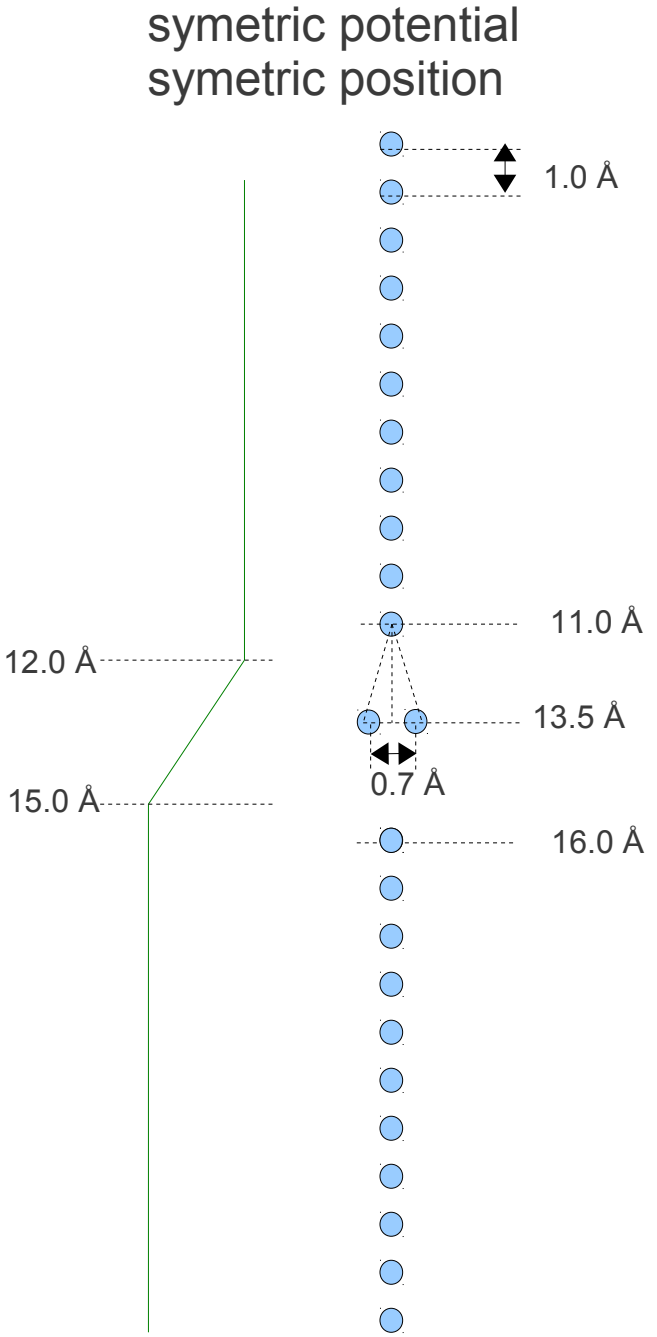


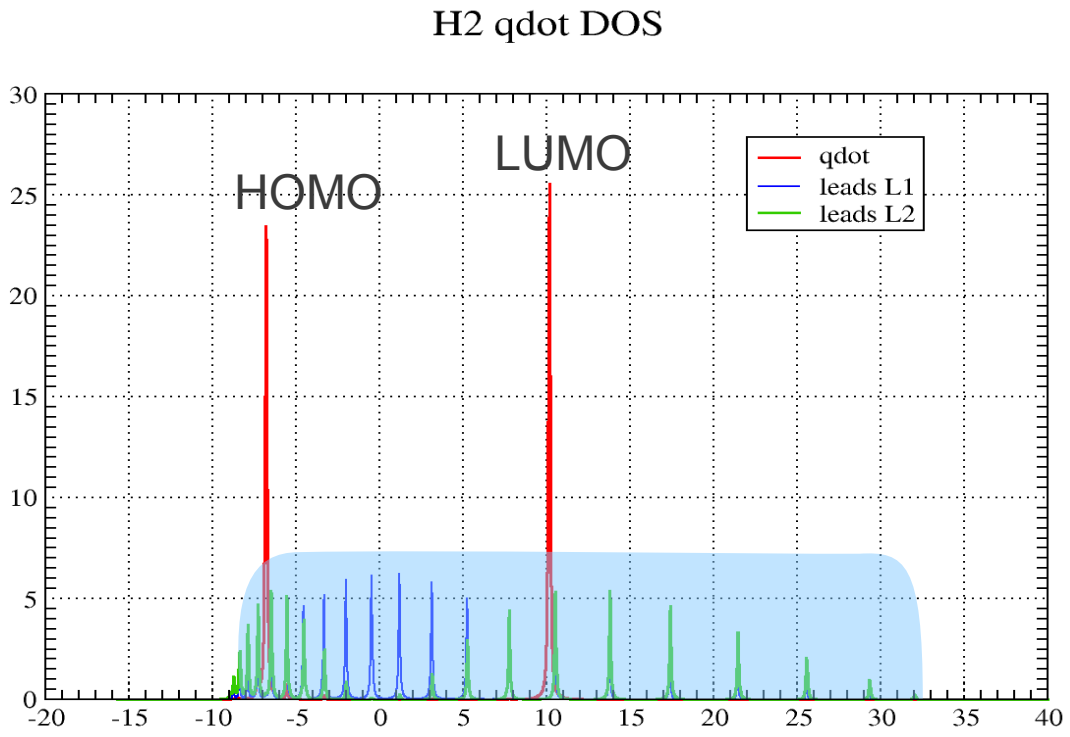
Example 1

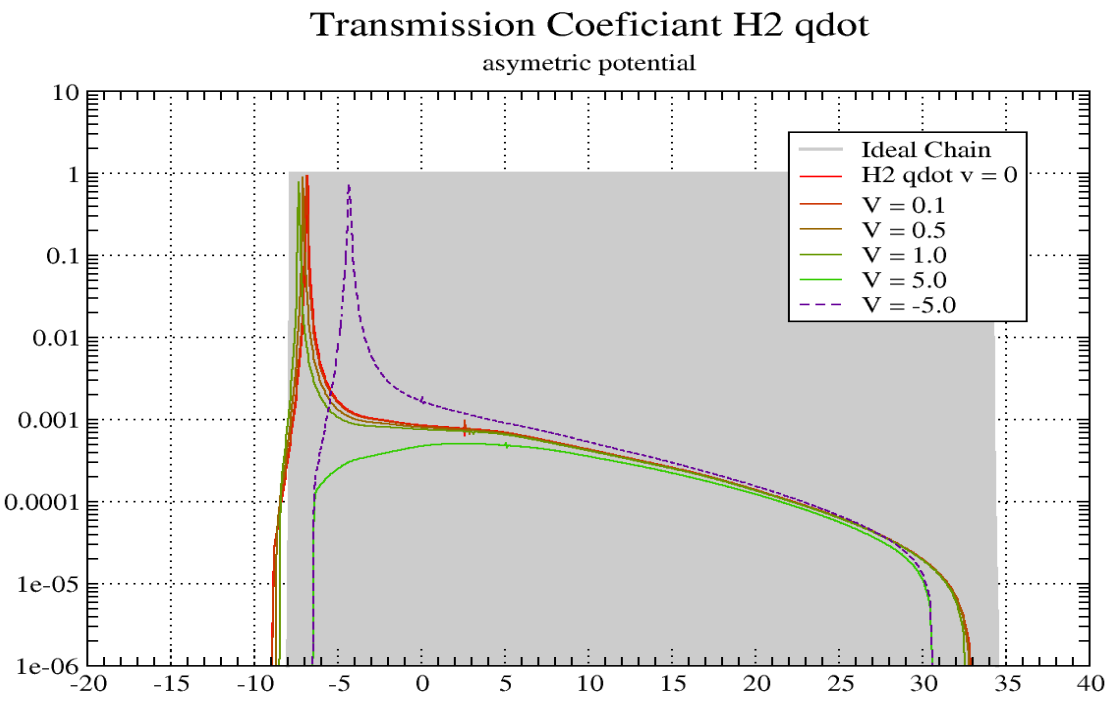
H_2 quantum dot in nonselfconsistent potential

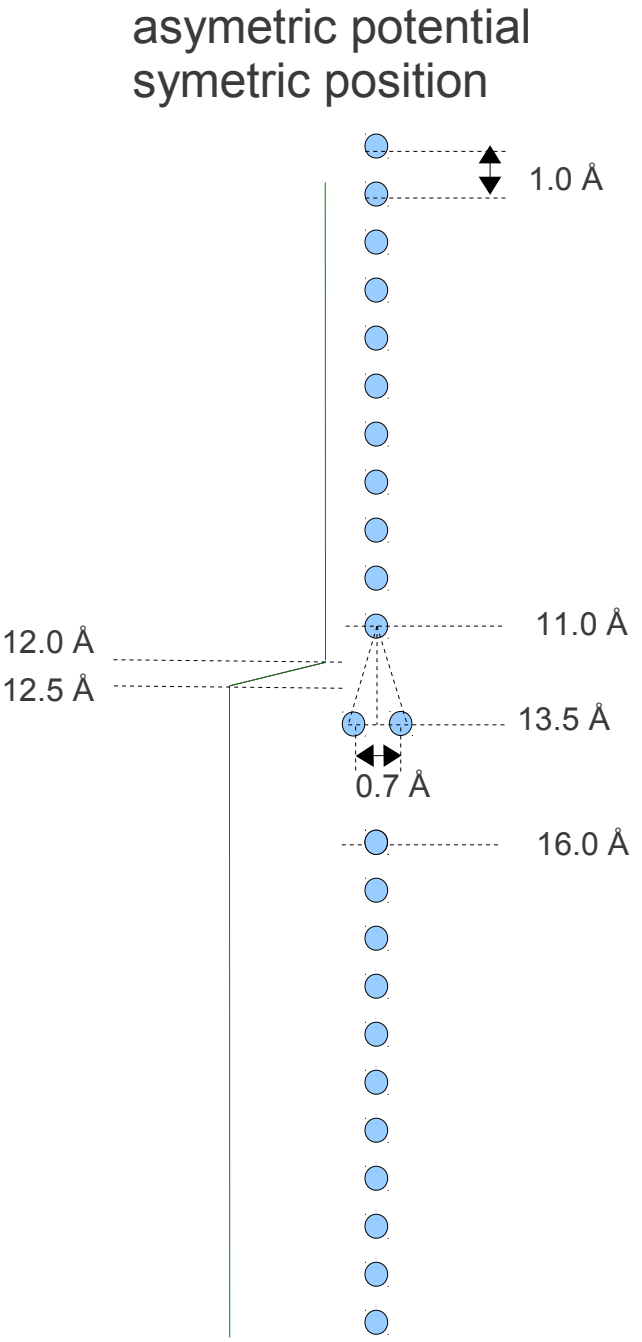

H2 qdot DOS
HOMO
LUMO
qdot
leads L1
leads L2


Transmission Coeficiant H2 qdot
symetric potential
Ideal Chain
H2 qdot v = 0
V = 0.1
V = 0.5
V = 1.0
V = 5.0


symetric potential
symetric position
1.0 Å
11.0 Å
12.0 Å
13.5 Å
0.7 Å
15.0 Å
16.0 Å


H2 qdot DOS
HOMO
LUMO
qdot
leads L1
leads L2

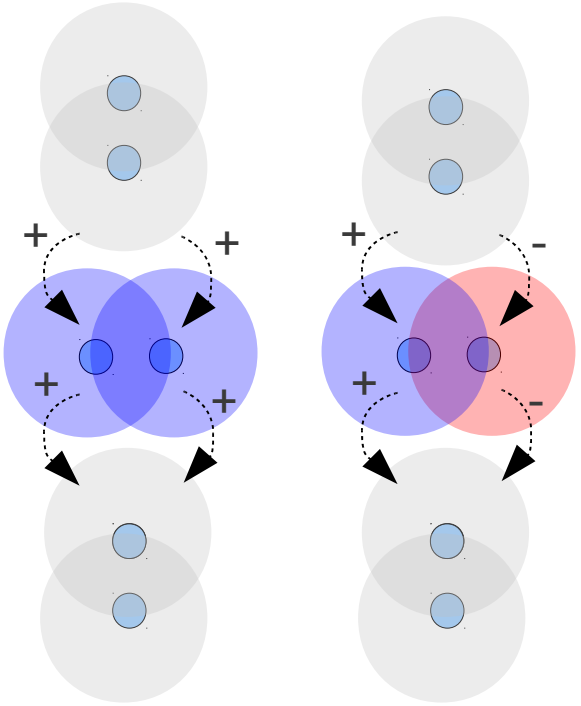

Transmission Coeficiant H2 qdot
asymetric potential
Ideal Chain
H2 qdot v = 0
V = 0.1
V = 0.5
V = 1.0
V = 5.0
V = -5.0


asymetric potential
symetric position
1.0 Å
12.0 Å
12.5 Å
11.0 Å
13.5 Å
0.7 Å
16.0 Å

H2 quantum dot (exlanation)

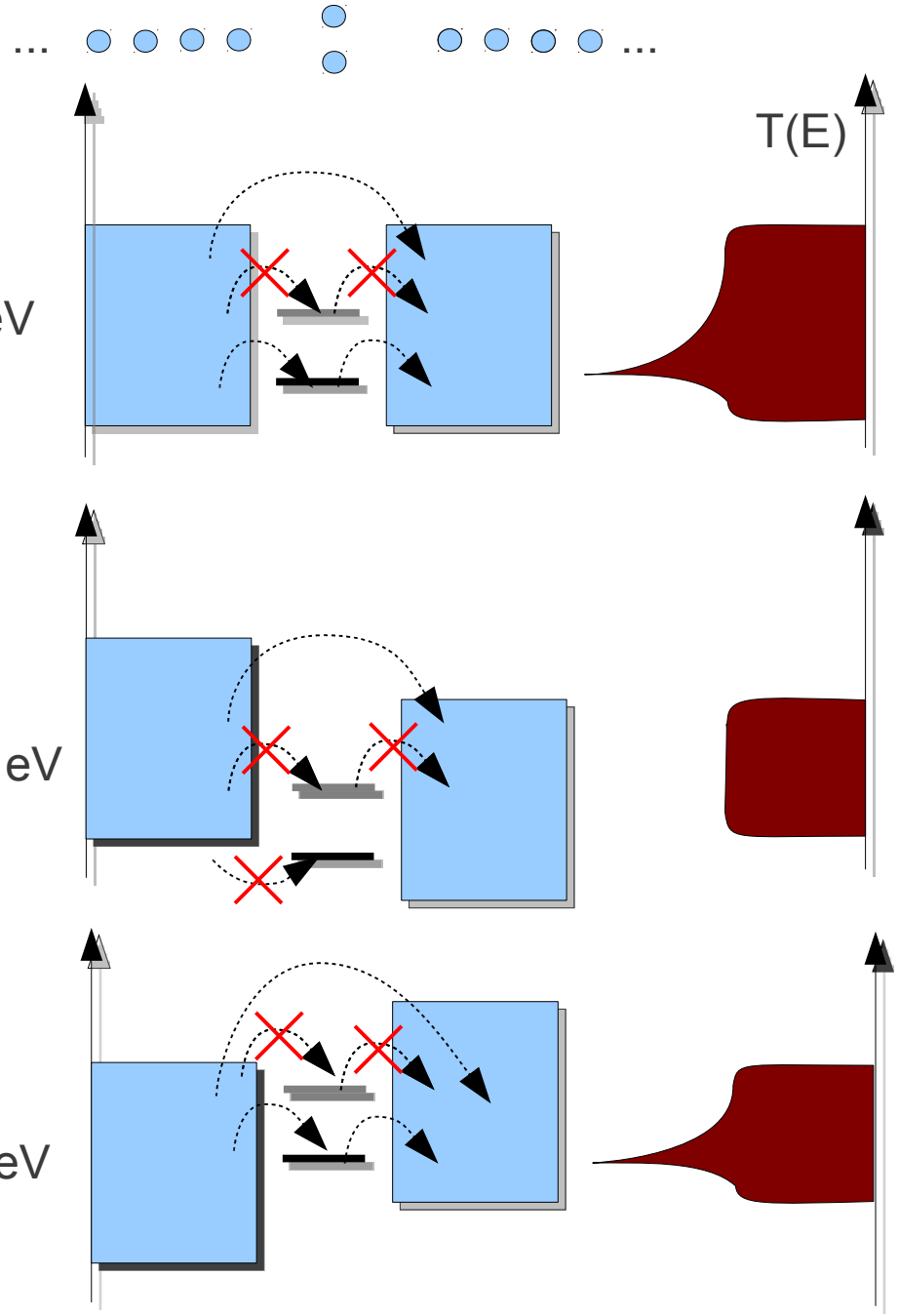
HOMO
bonding

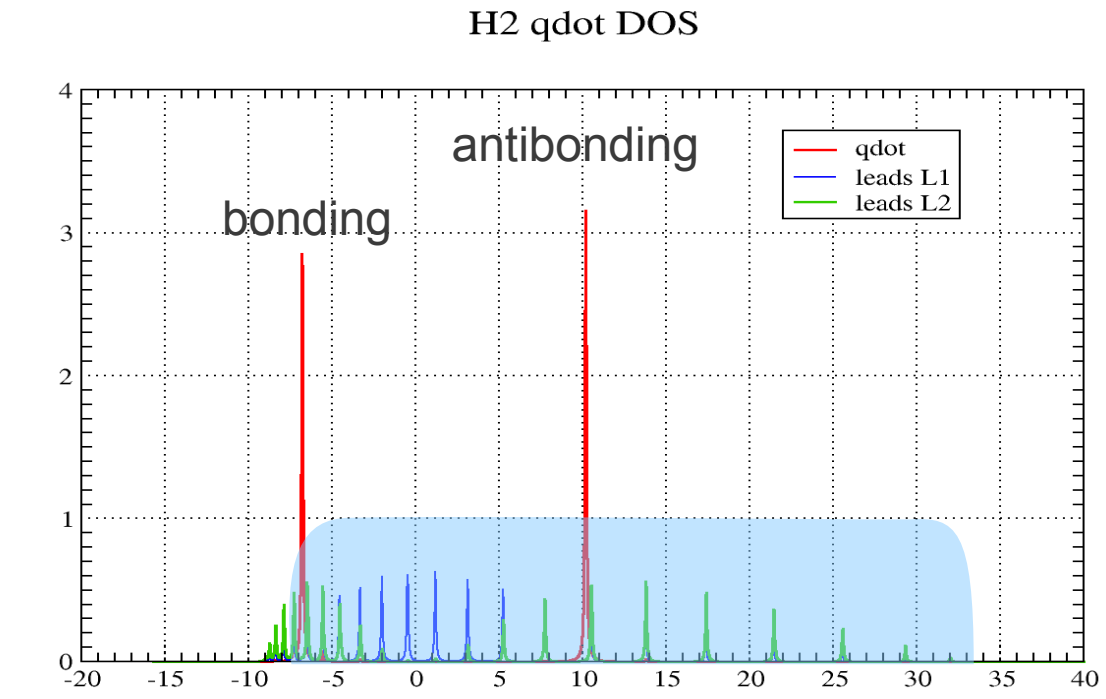
LUMO
antibonding

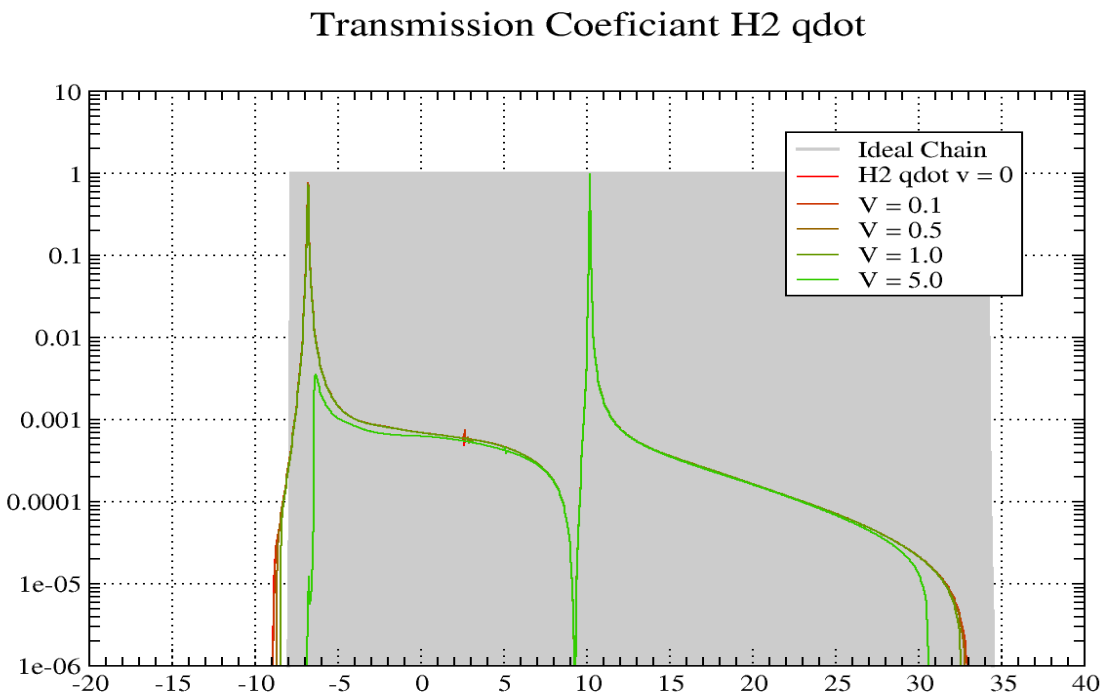


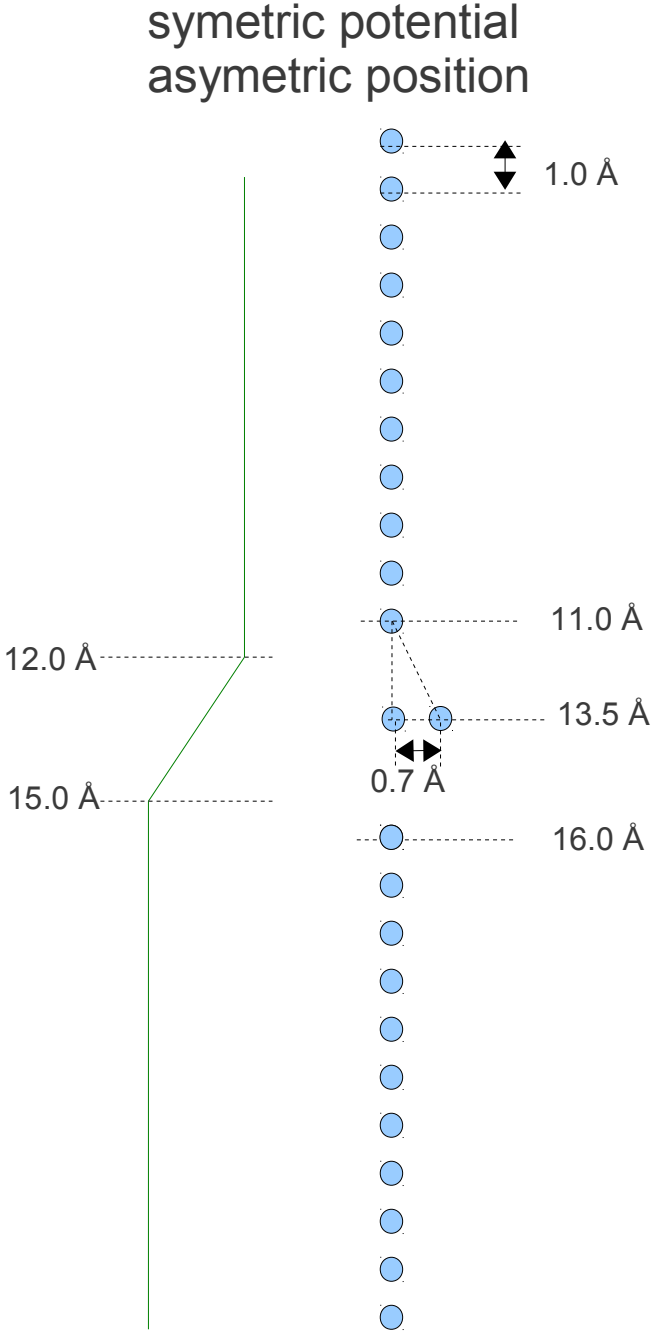
$t_{12} \sim \int s \cdot (s + s) = 0$

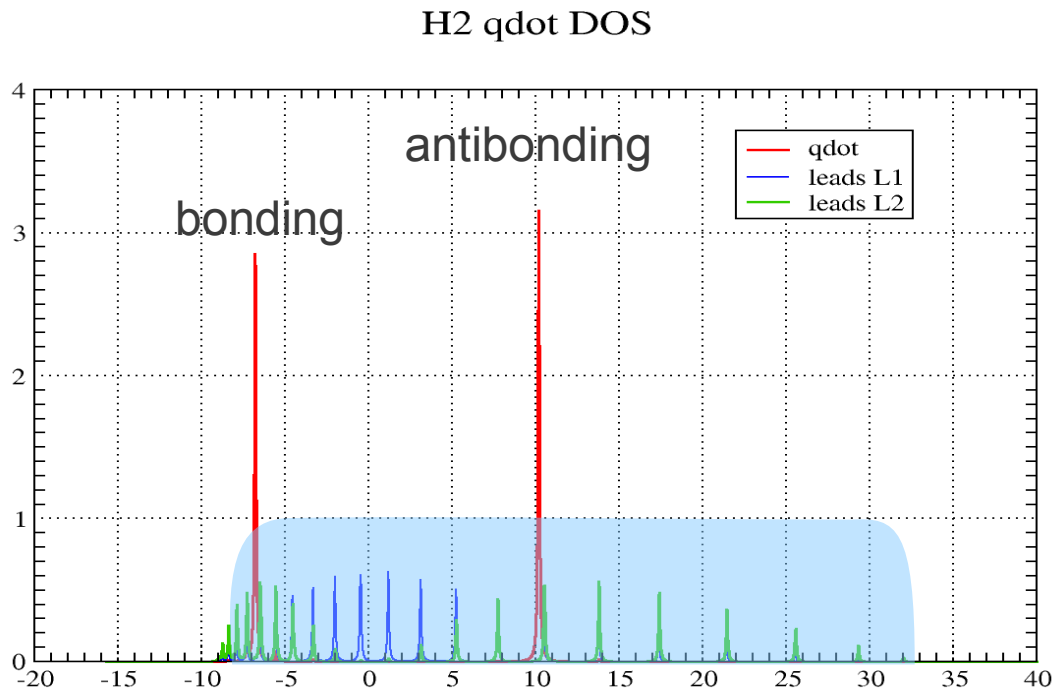
$t_{12} \sim \int s \cdot (s - s) = 0$

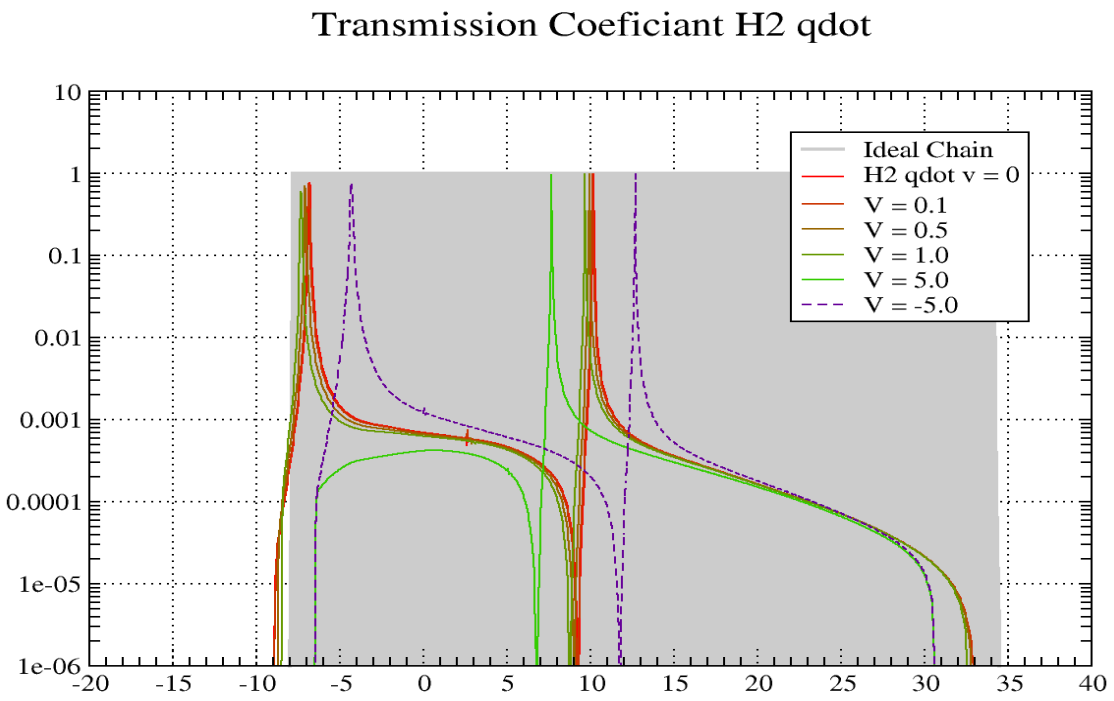


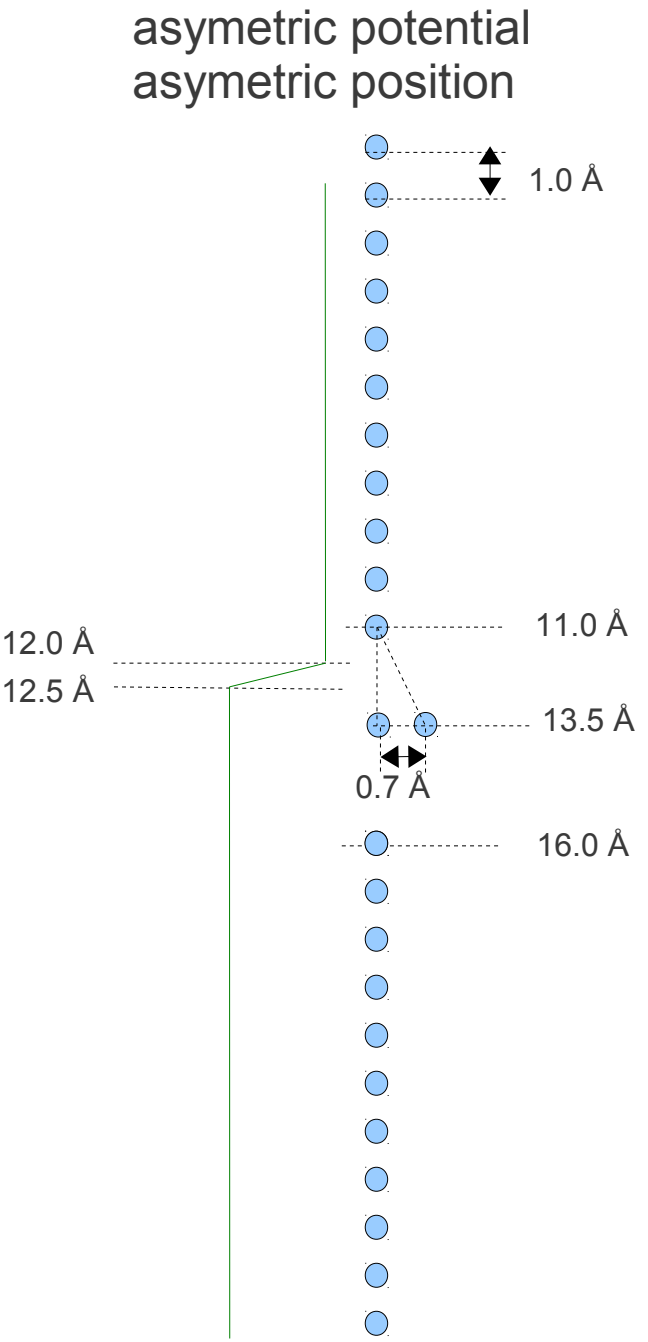

H2 qdot DOS
antibonding
bonding
qdot
leads L1
leads L2


Transmission Coeficiant H2 qdot
Ideal Chain
H2 qdot v = 0
V = 0.1
V = 0.5
V = 1.0
V = 5.0


symetric potential
asymetric position
1.0 Å
11.0 Å
12.0 Å
13.5 Å
0.7 Å
15.0 Å
16.0 Å


H2 qdot DOS
antibonding
bonding
qdot
leads L1
leads L2

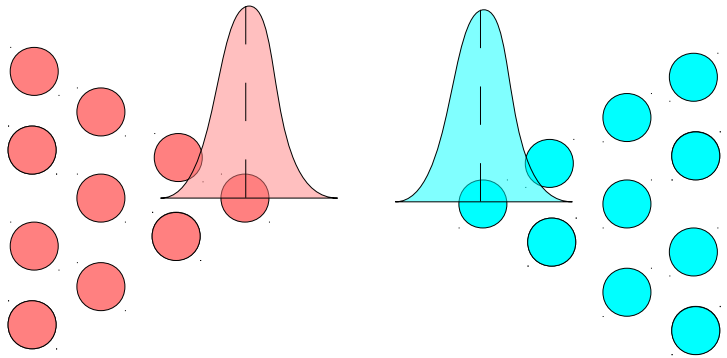

Transmission Coeficiant H2 qdot
Ideal Chain
H2 qdot v = 0
V = 0.1
V = 0.5
V = 1.0
V = 5.0
V = -5.0


asymetric potential
asymetric position
1.0 Å
11.0 Å
12.0 Å
12.5 Å
13.5 Å
0.7 Å
16.0 Å

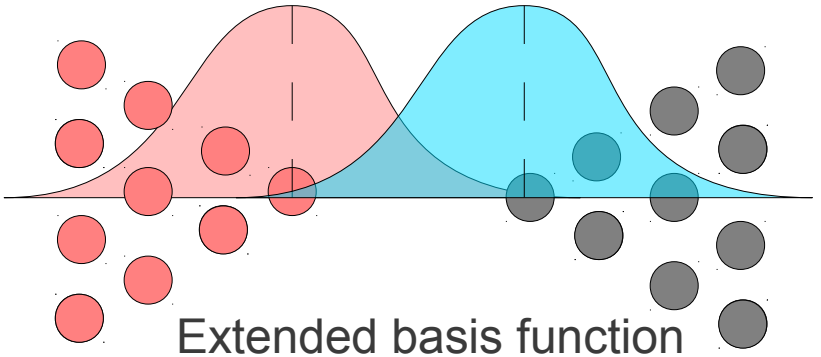
Example 2

Braking Gold Chain
width extendet
hopping

extended hopping



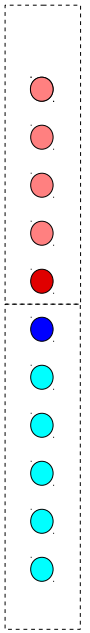
Original basis function

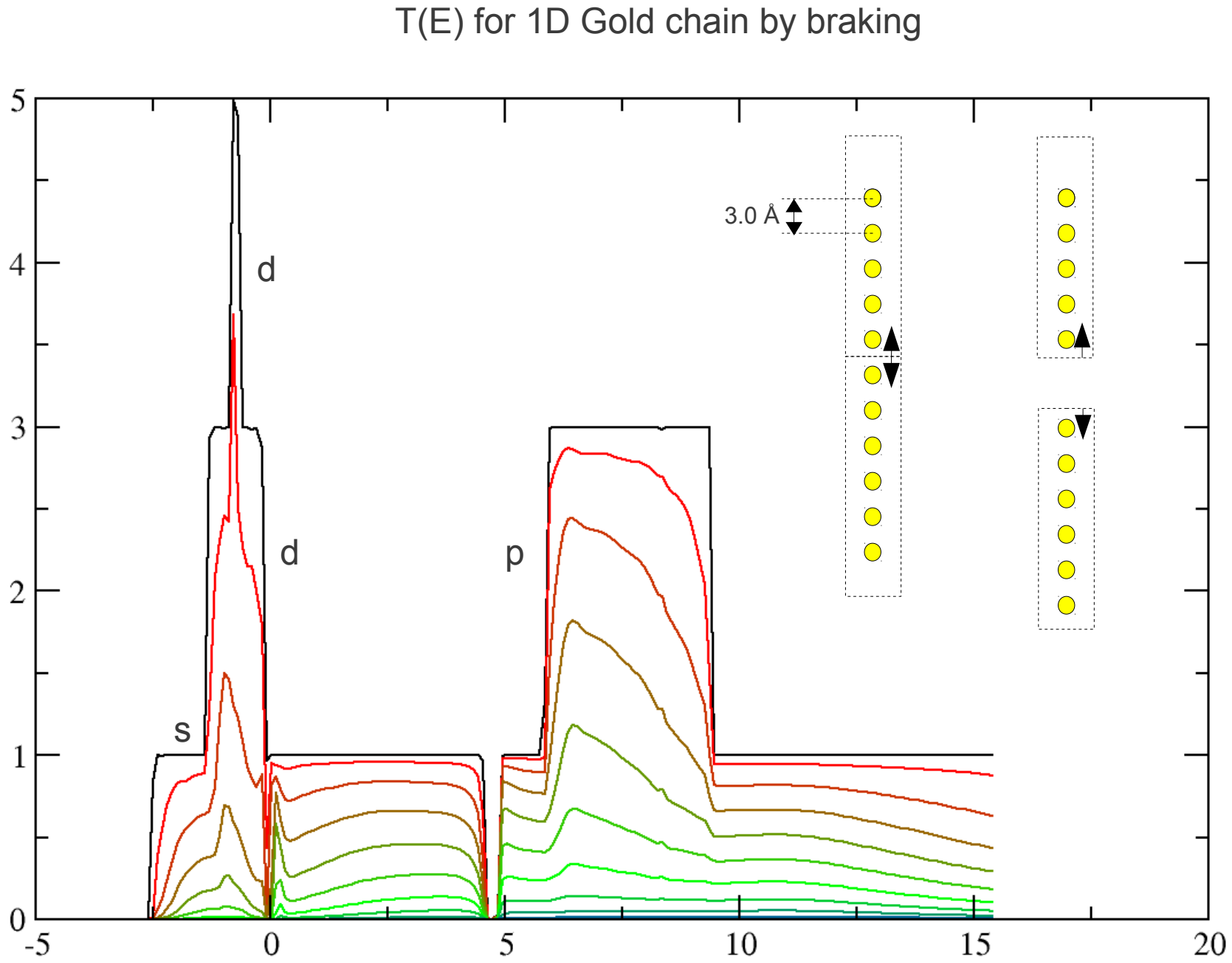


Extended basis function
in apex region

This is replaced to H and S matrix
in apex region before
before construction of Green's function

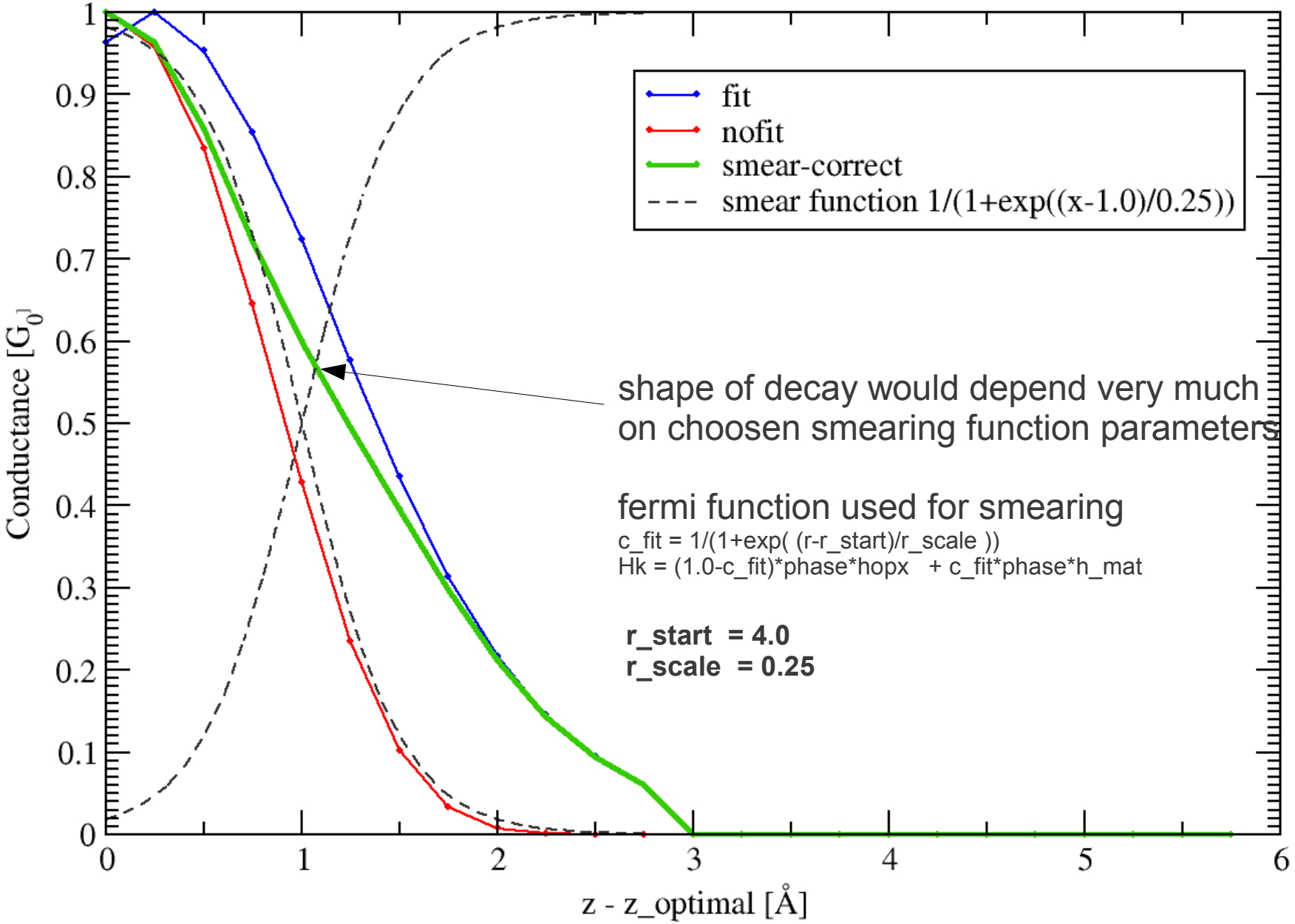
```
interaction.optional   [----]  1 L:[  1+11  12/ 13] *(650 / 686b)=    32 0x20
0                      ! ncell sample1
12                     ! total number of atoms in the sample1
1                      ! number of intervals defining the sample1
1  12                  ! atom1 atom2 of the interval
1                                ! number of atoms in tip1
6      ! list of atoms in the tip1
0                                ! ncell sample1
12                               ! total number of atoms in the sample2
1                                ! number of intervals defining the sample2
1  12                           ! atom1 atom2 of the interval
1                                ! number of atoms in tip2
7      ! list of atoms in the tip2
```




T(E) for 1D Gold chain by braking
5
4
3
2
1
0
-5
0
5
10
15
20
s
d
d
p
3.0 Å

hopping fit smear Au-Chain 3.0Å

in +2,0 eV from fermi level



shape of decay would depend very much on choosen smearing function parameters

fermi function used for smearing

c_fit = 1/(1+exp((r-r_start)/r_scale))

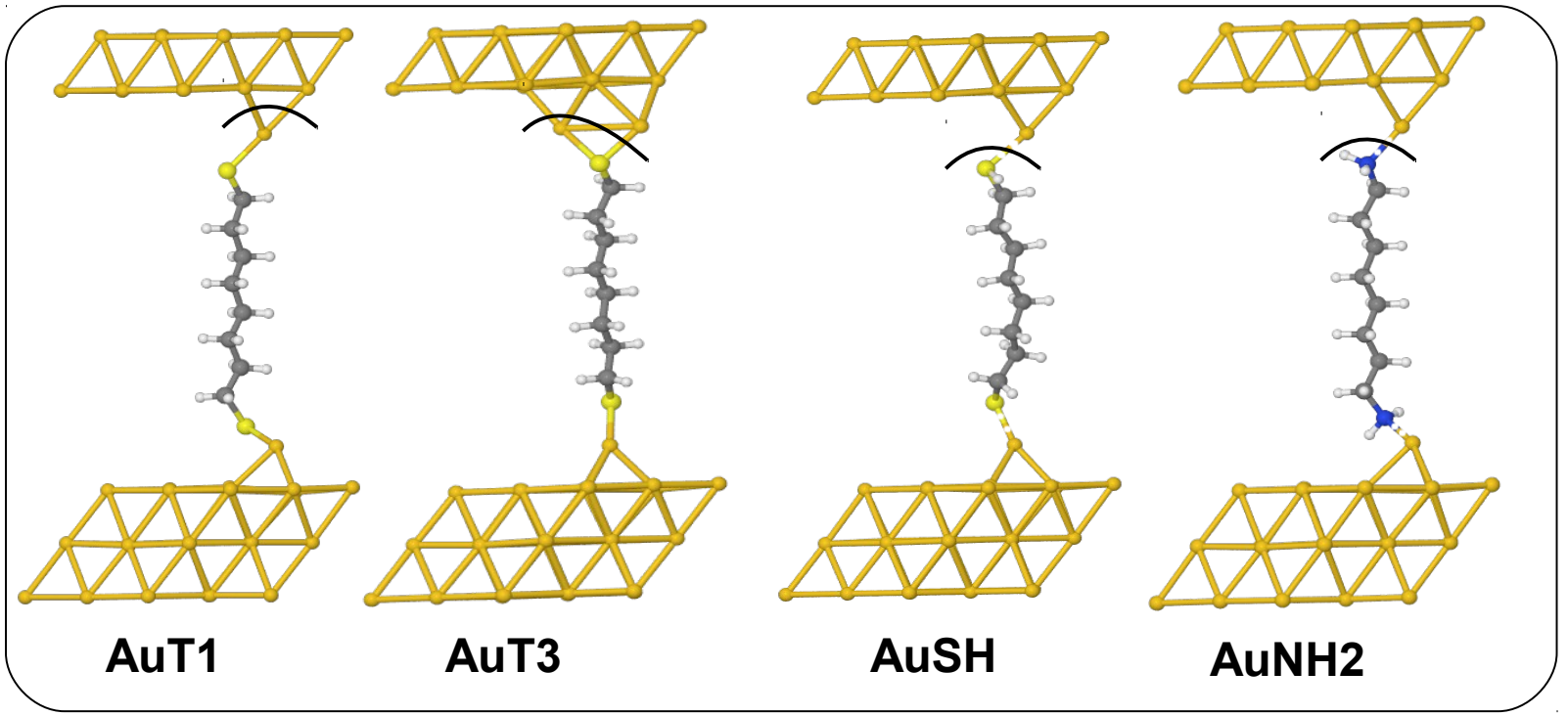
Hk = (1.0-c_fit)*phase*hopx + c_fit*phase*h_mat

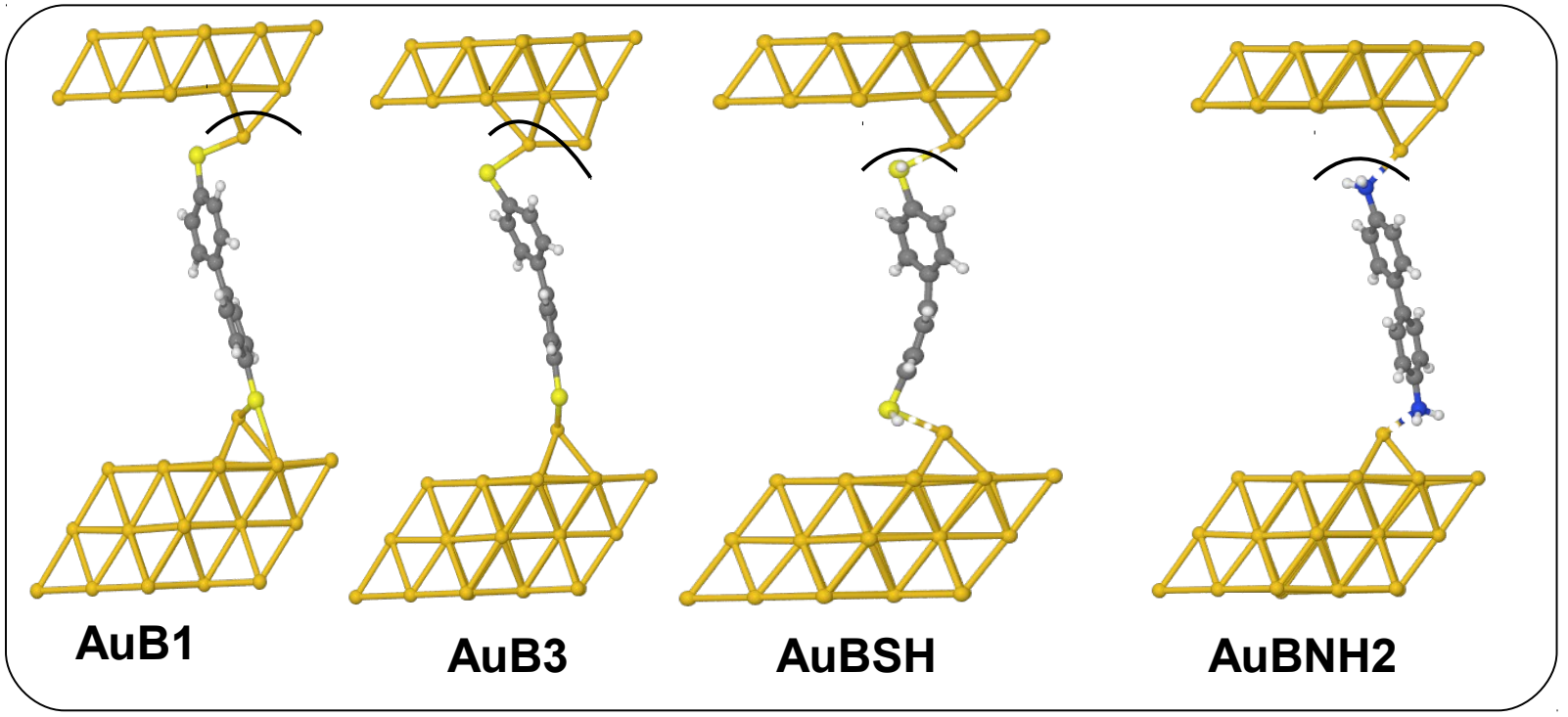
r_start = 4.0

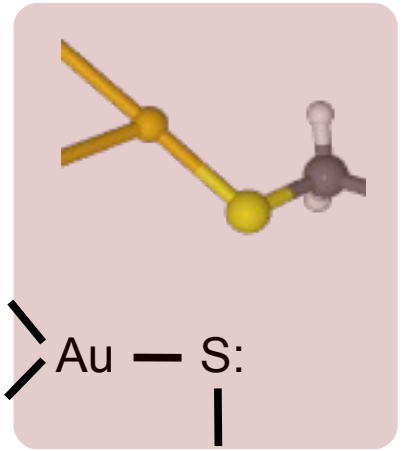
r_scale = 0.25

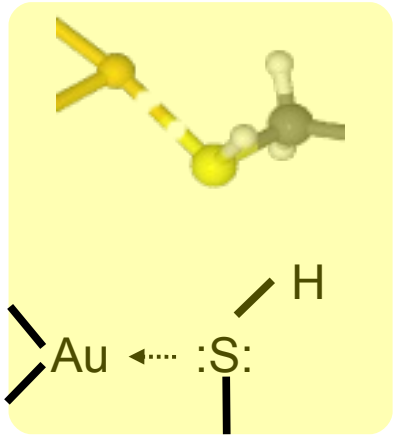
Example 3

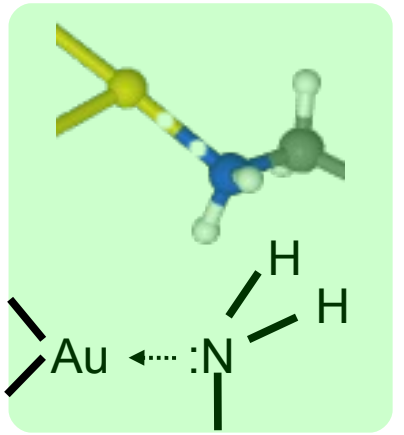
Conductance of molecules

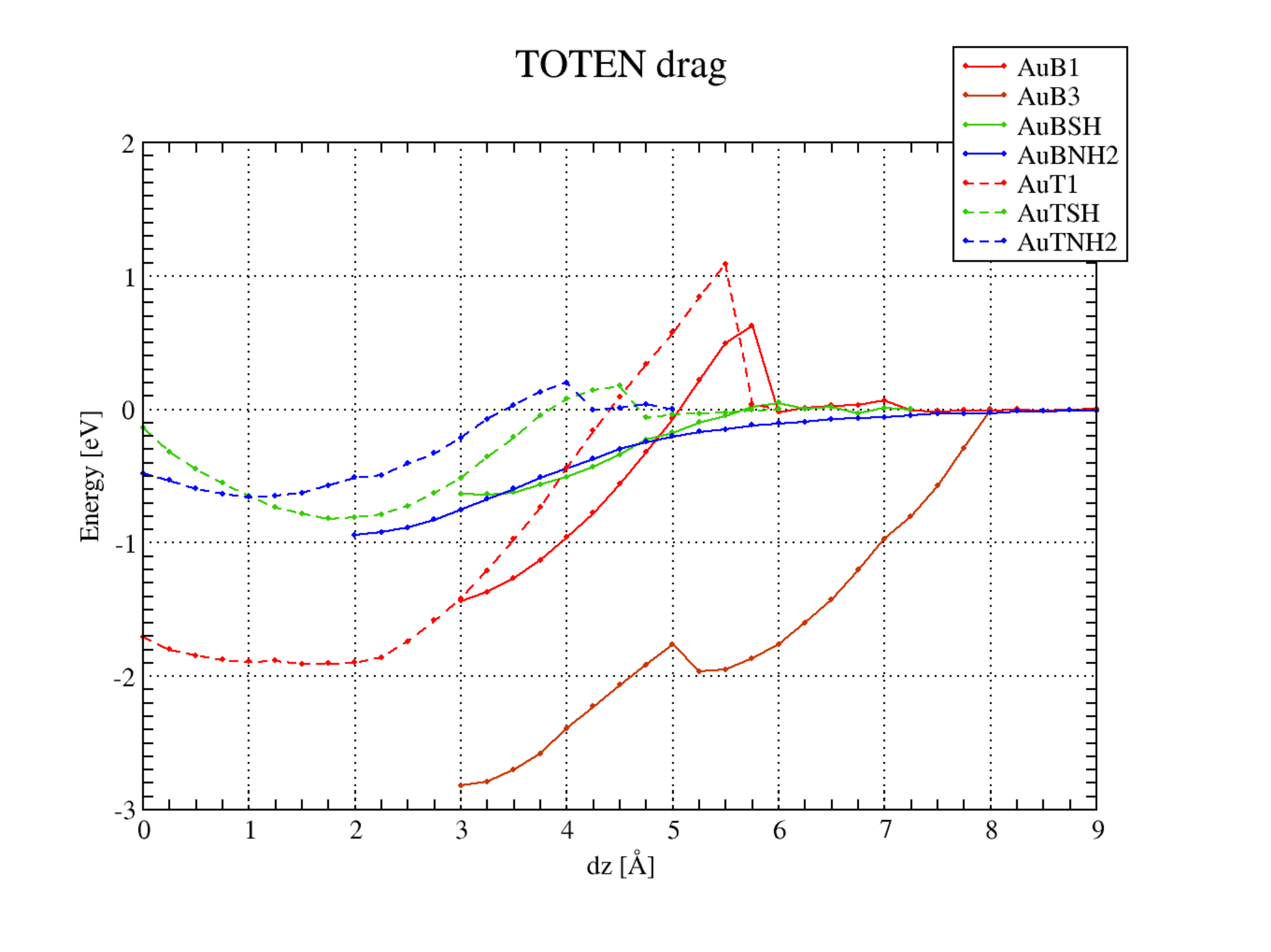

AuT1
AuT3
AuSH
AuNH2

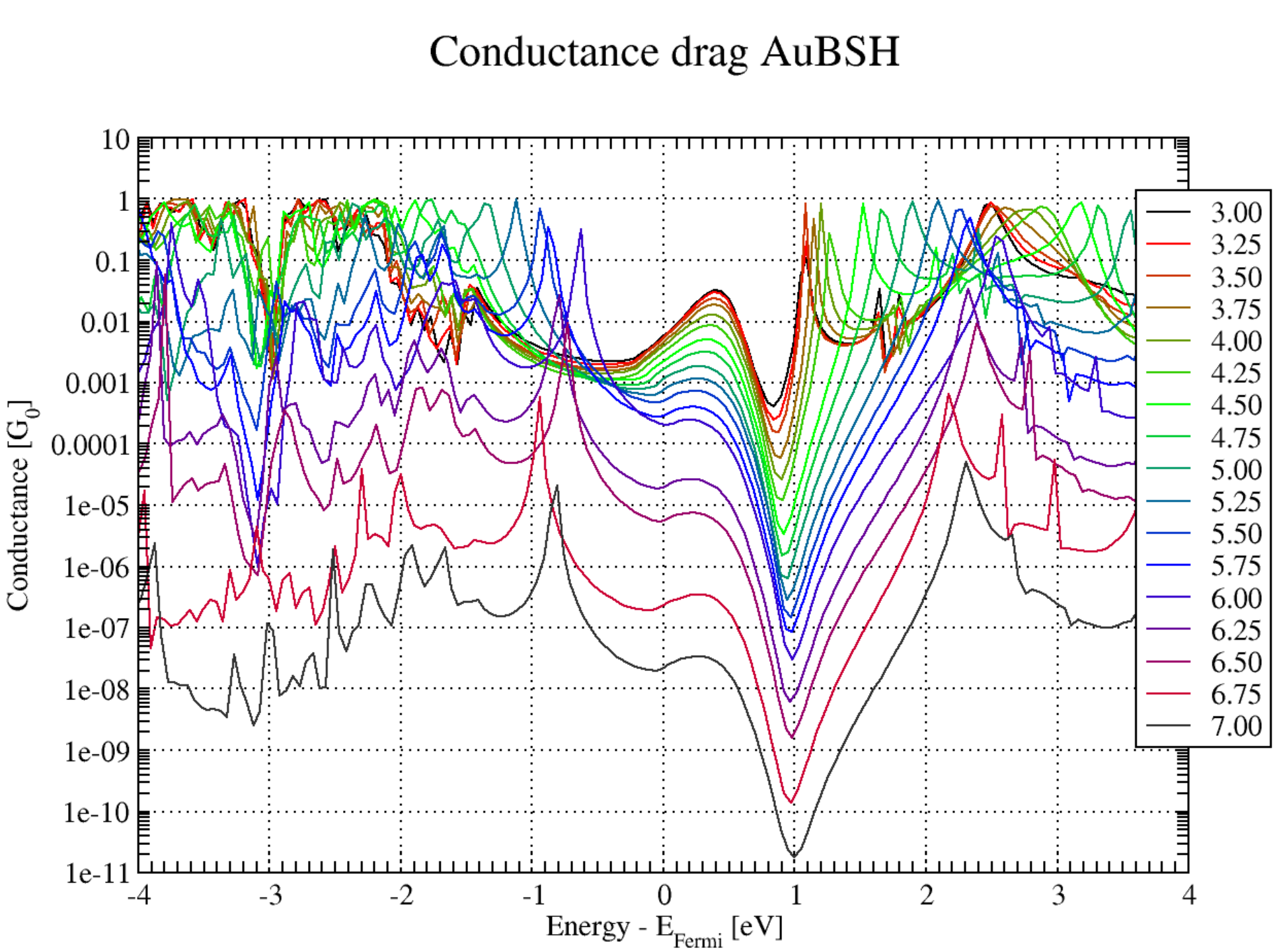

AuB1
AuB3
AuBSH
AuBNH2

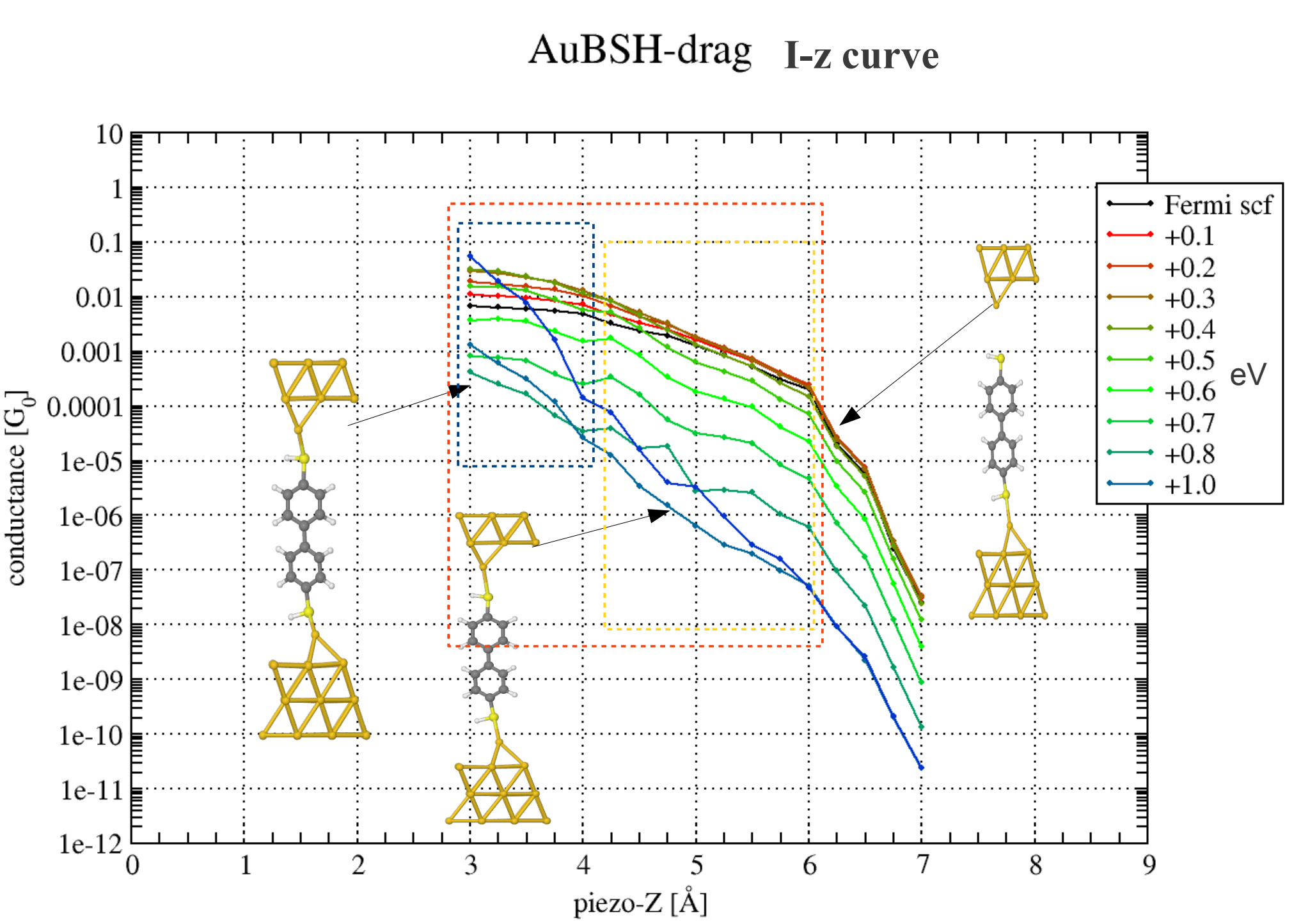

Au
S:


H
Au
:S:


H
H
Au
:N


TOTEN drag
AuB1
AuB3
AuBSH
AuBNH2
AuT1
AuTSH
AuTNH2
Energy [eV]
dz [Å]
2
1
0
-1
-2
-3
0
1
2
3
4
5
6
7
8
9


Conductance drag AuBSH
Conductance [G0]
Energy - EFermi [eV]
10
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
1e-08
1e-09
1e-10
1e-11
-4
-3
-2
-1
0
1
2
3
4
3.00
3.25
3.50
3.75
4.00
4.25
4.50
4.75
5.00
5.25
5.50
5.75
6.00
6.25
6.50
6.75
7.00


AuBSH-drag I-z curve
conductance [G0]
piezo-Z [Å]
Fermi scf
+0.1
+0.2
+0.3
+0.4
+0.5
+0.6
+0.7
+0.8
+1.0
eV