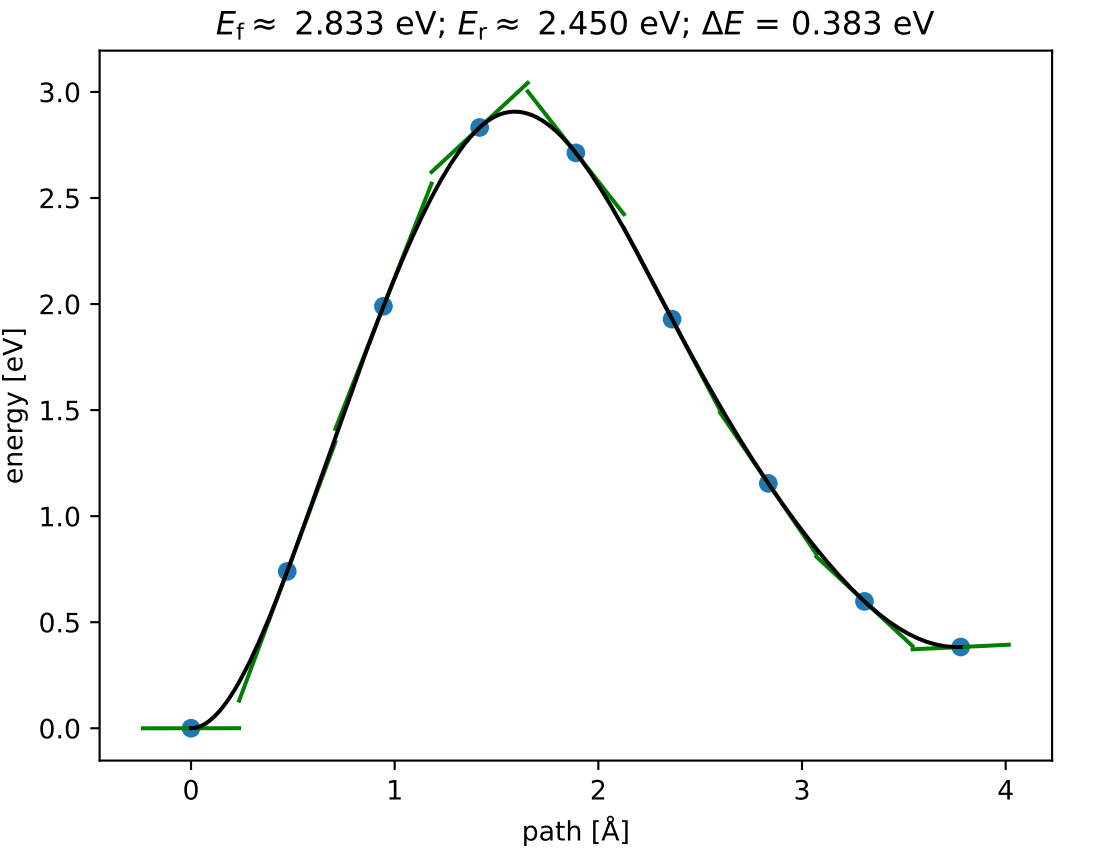
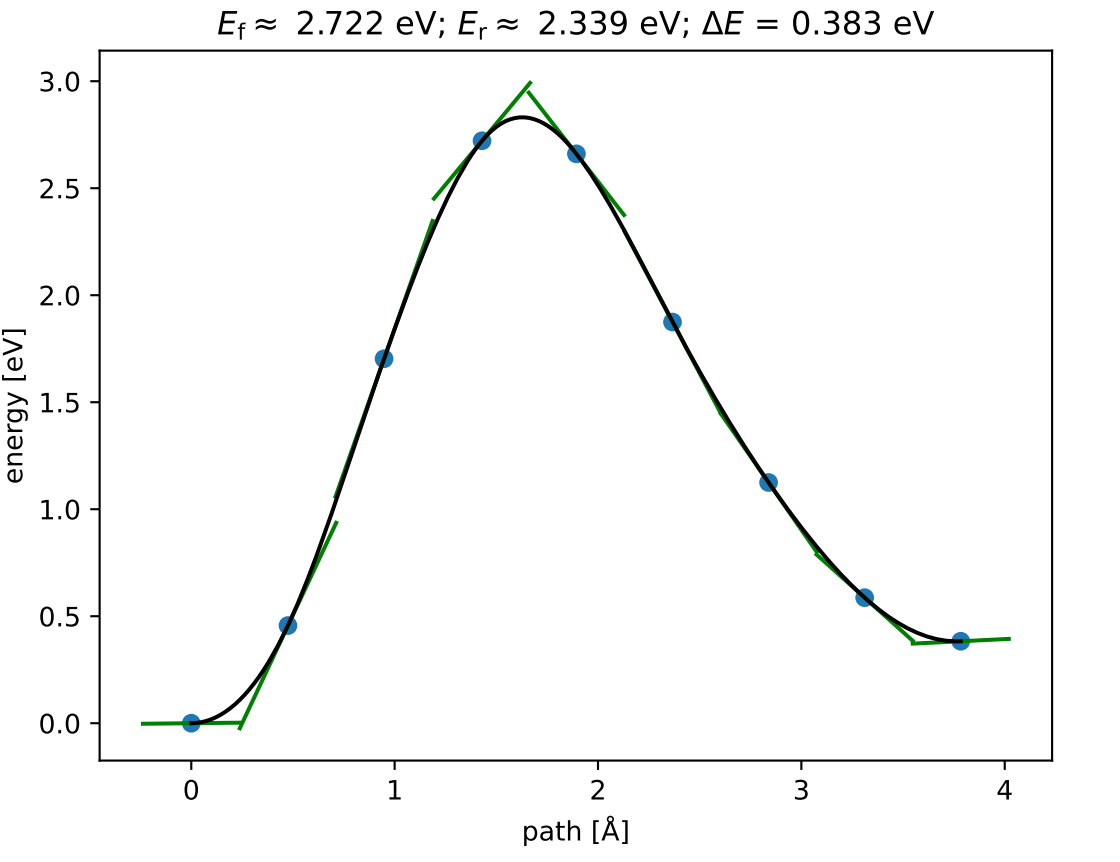

$E_f \approx$ 2.833 eV; $E_r \approx$ 2.450 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
1
2
3
4


$E_f \approx$ 2.722 eV; $E_r \approx$ 2.339 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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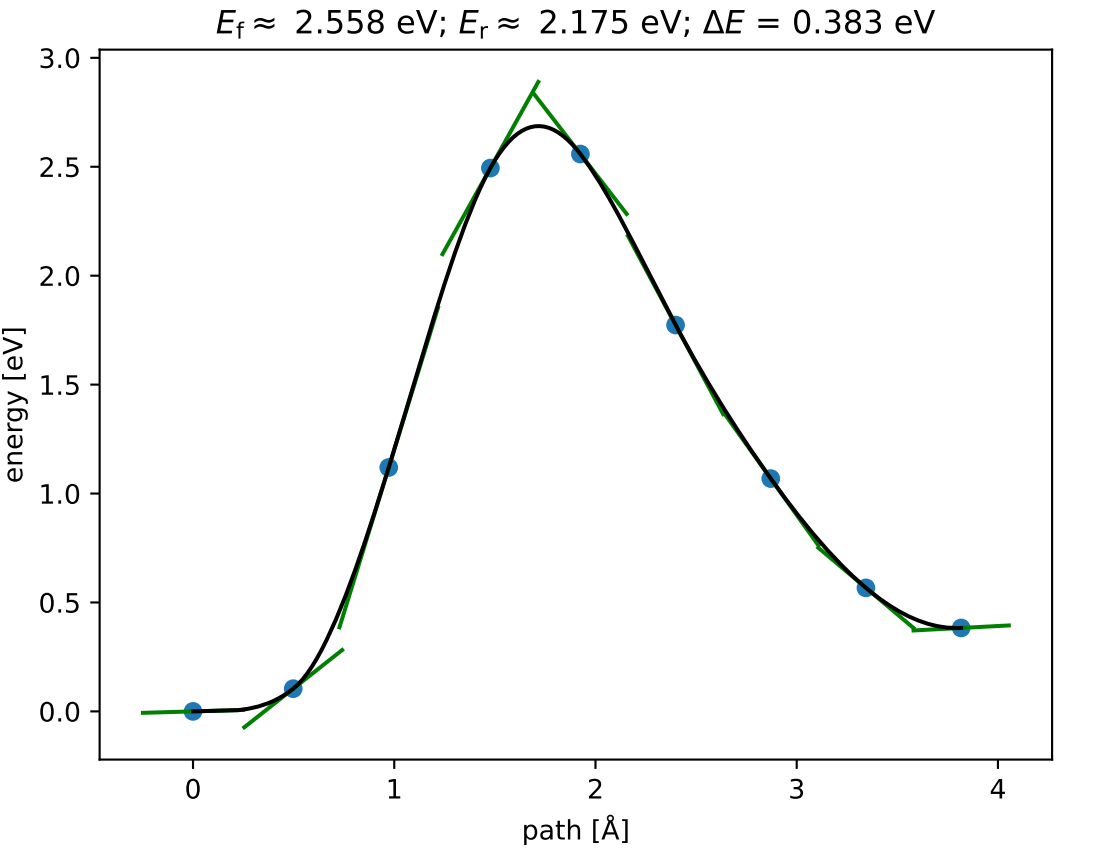
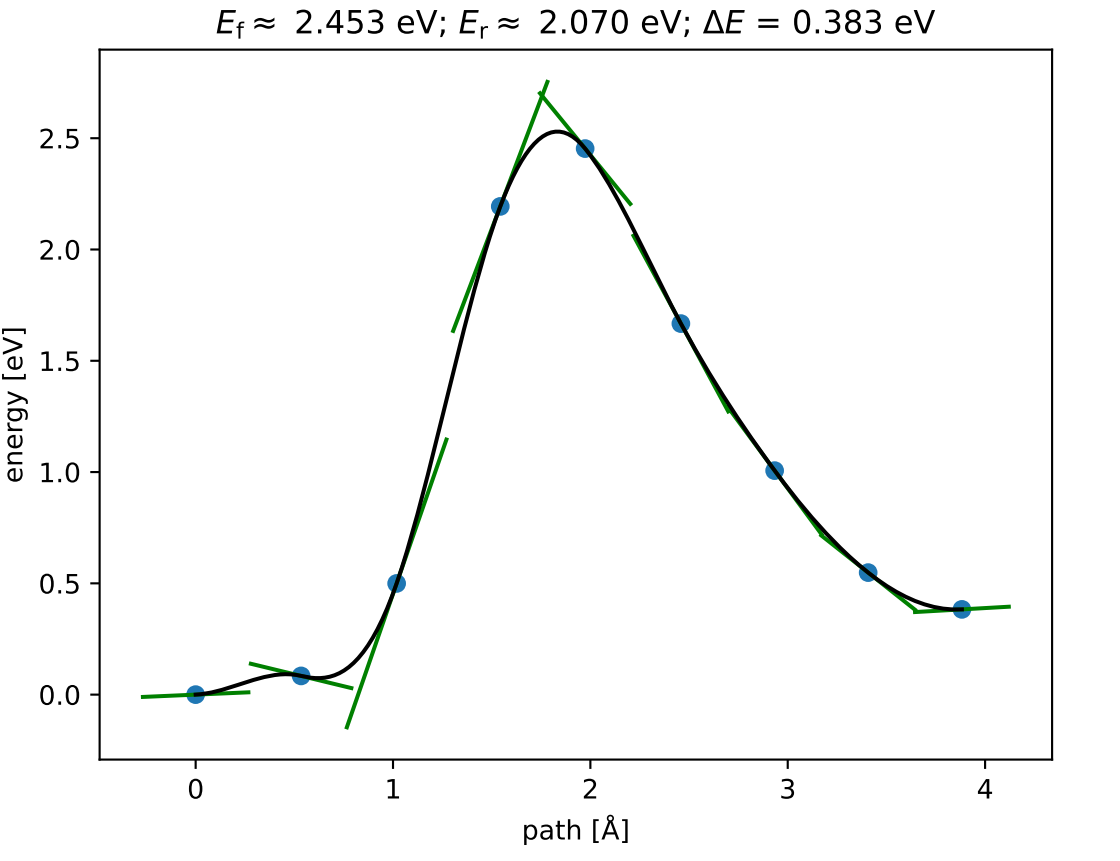
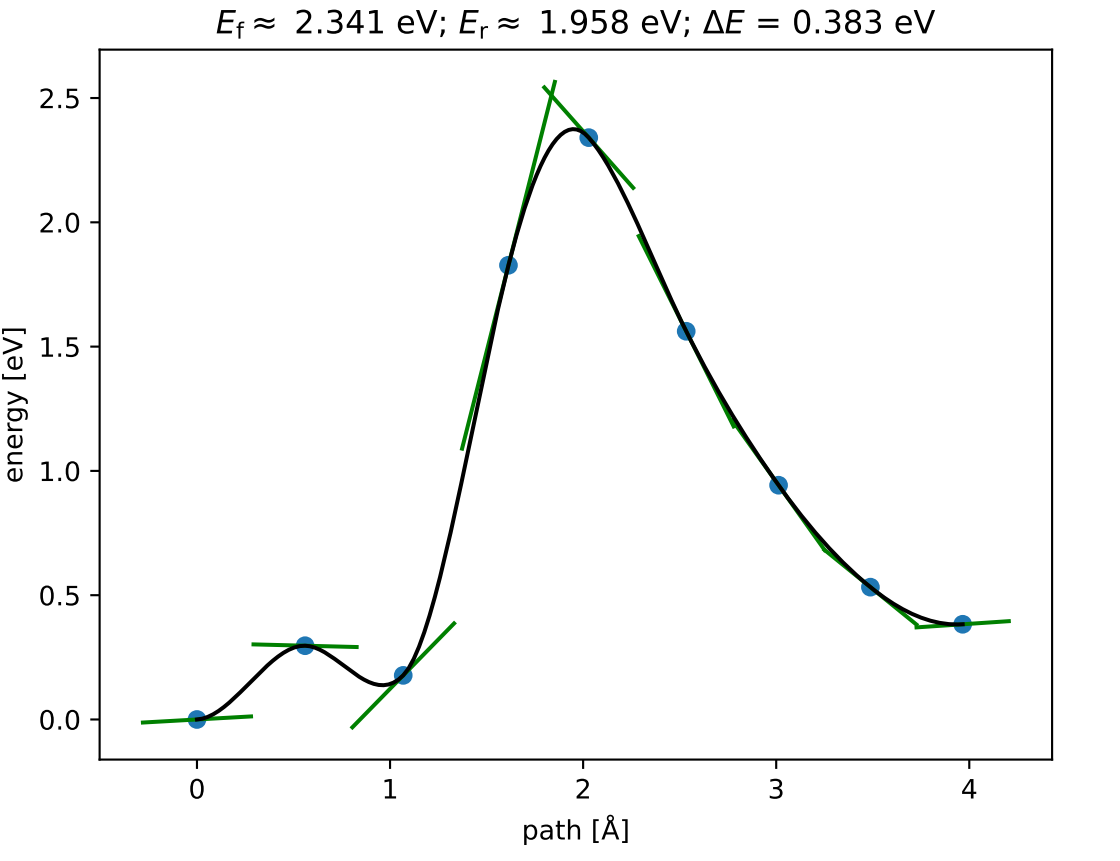
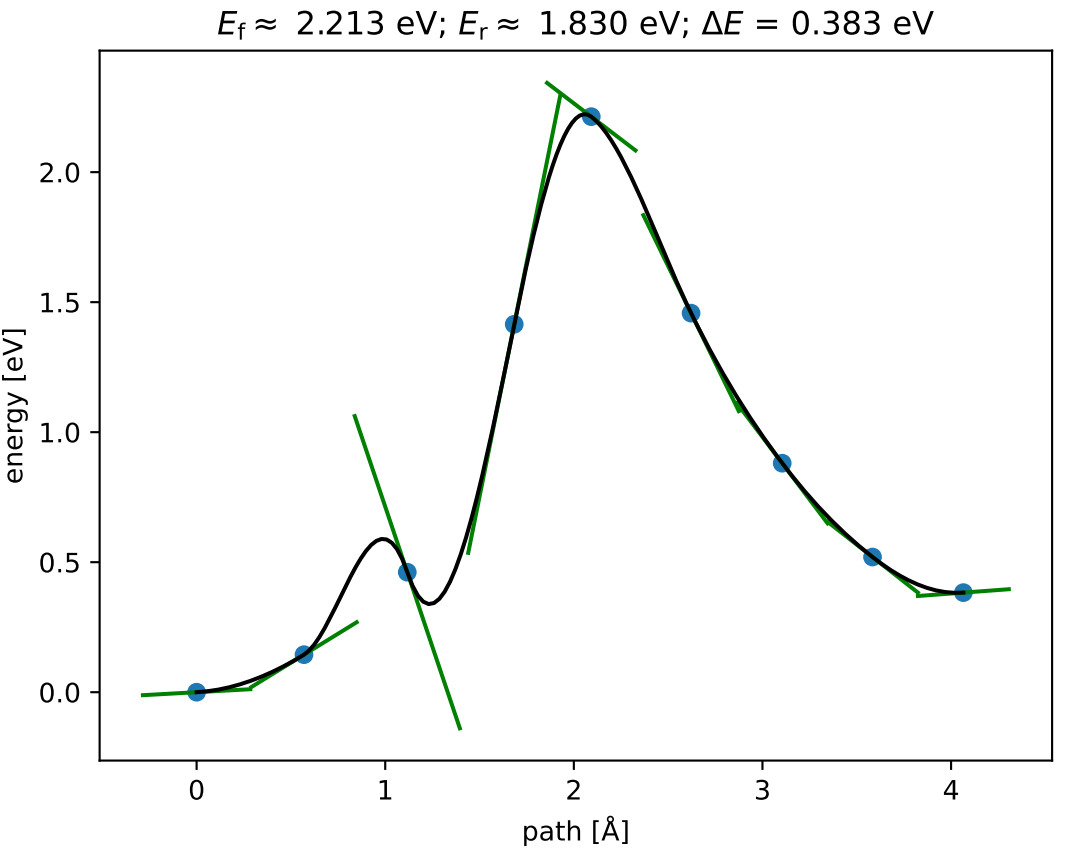
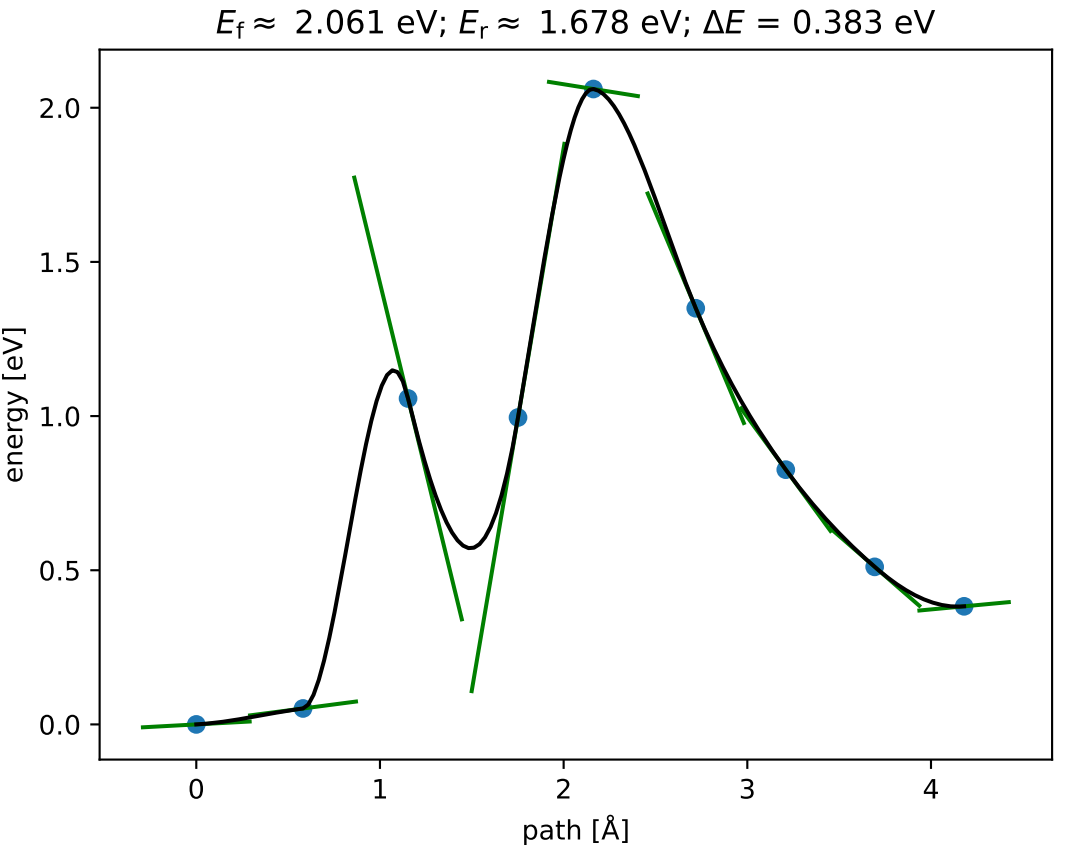
0.5
1.0
1.5
2.0
2.5
3.0
0
1
2
3
4

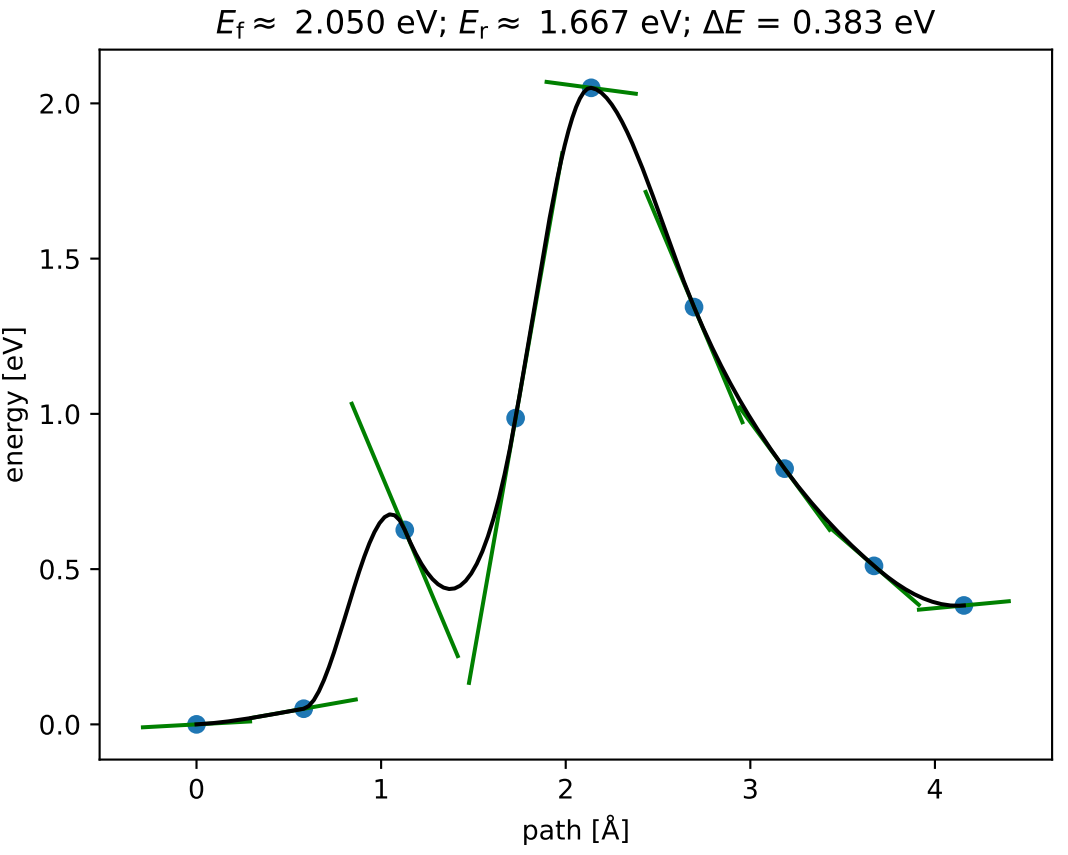

$E_f \approx$ 2.558 eV; $E_r \approx$ 2.175 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
1
2
3
4

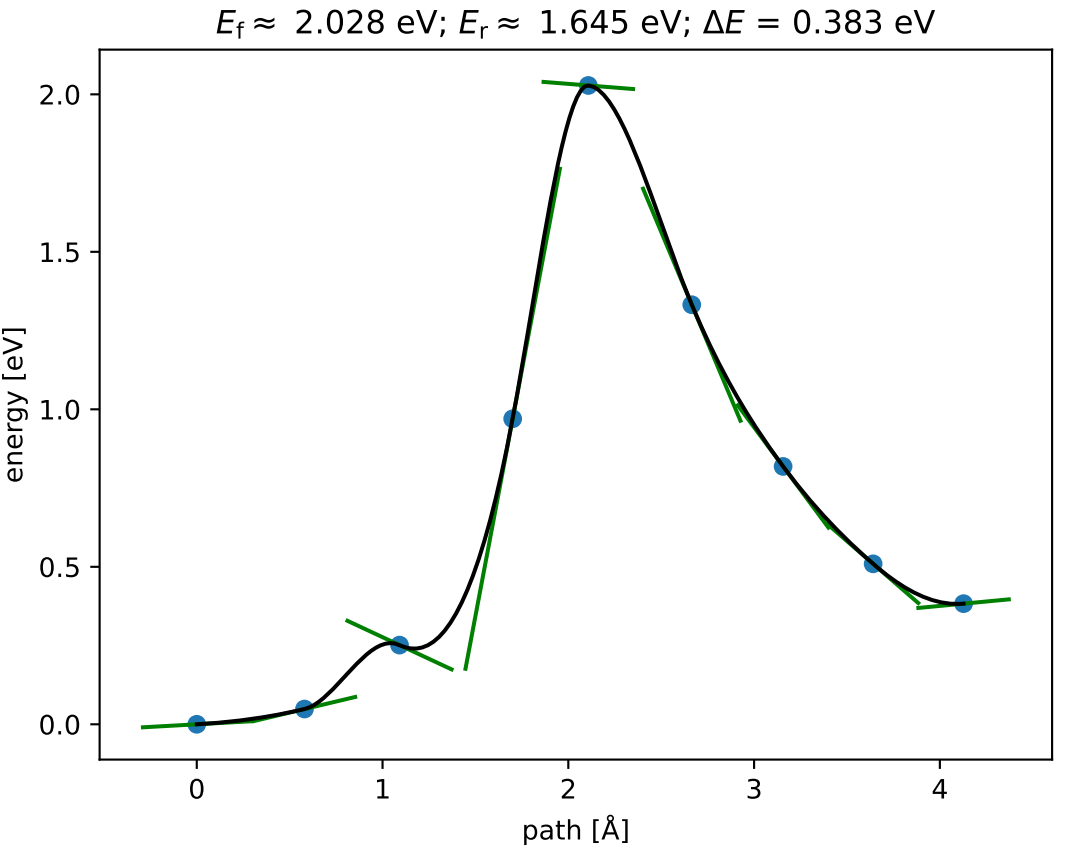

$E_f \approx$ 2.453 eV; $E_r \approx$ 2.070 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
2.5
0
1
2
3
4

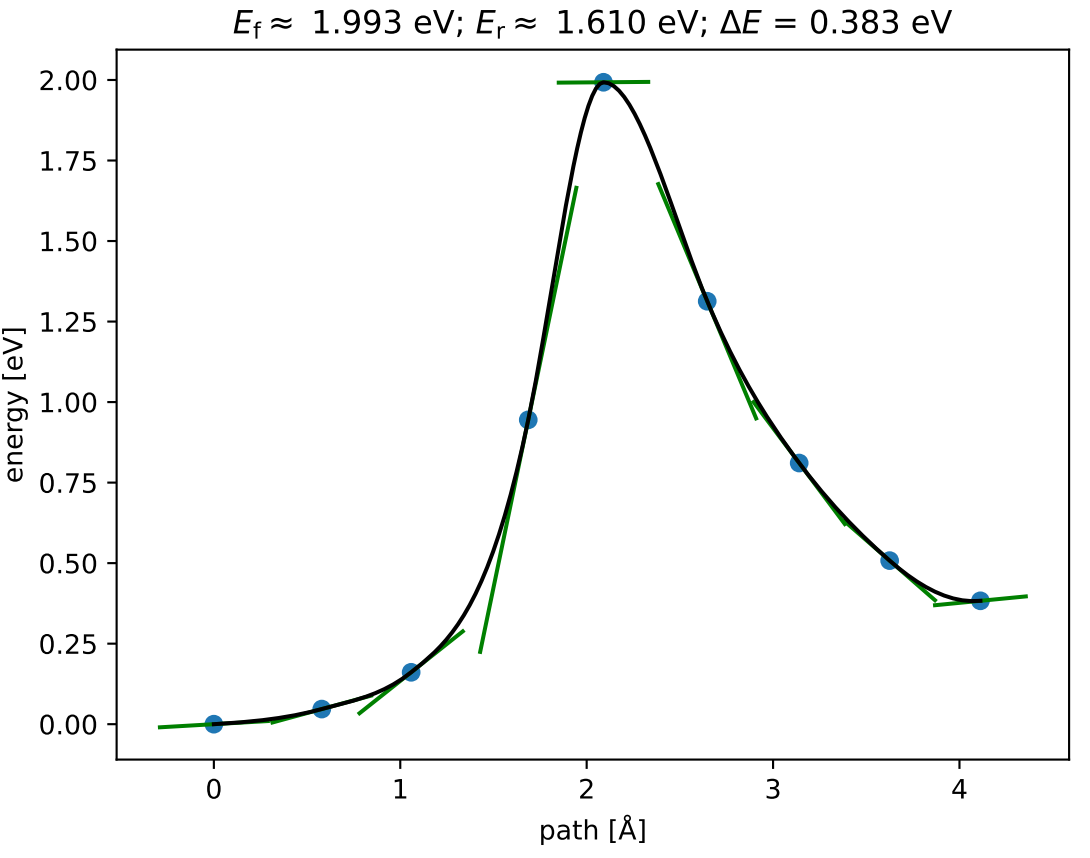

$E_f \approx$ 2.341 eV; $E_r \approx$ 1.958 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
2.5
0
1
2
3
4

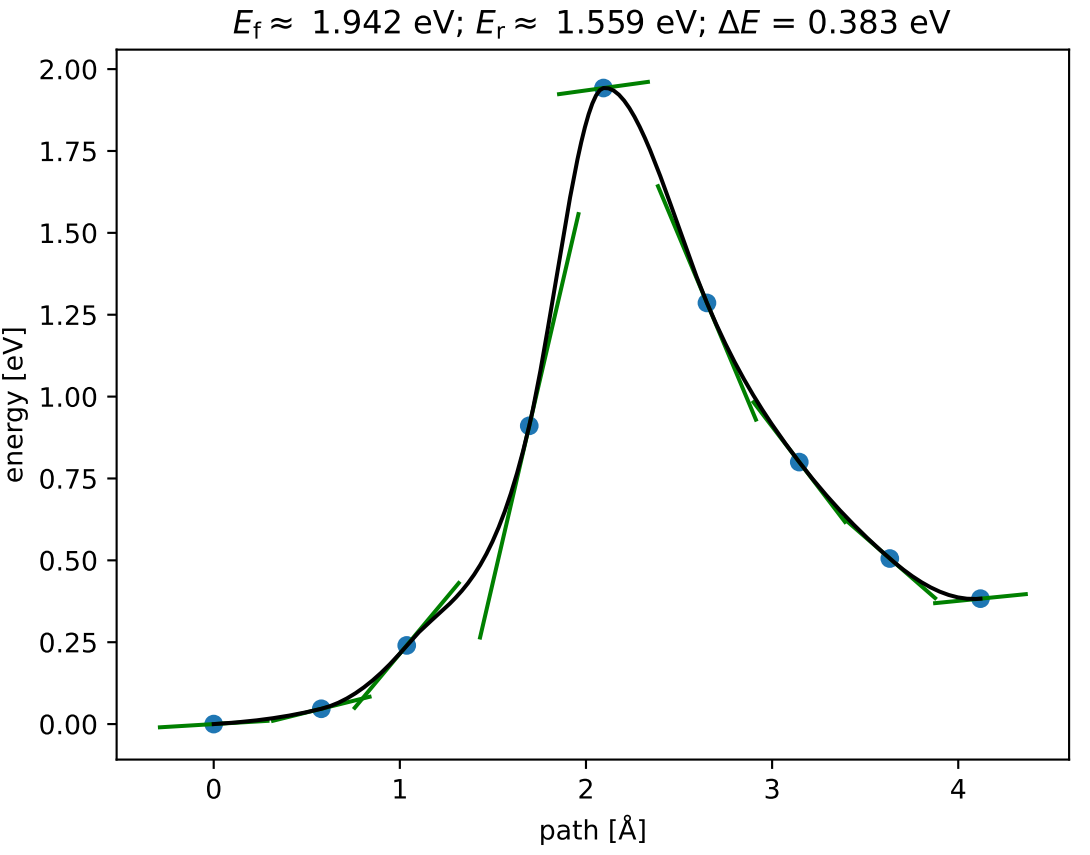

$E_f \approx$ 2.213 eV; $E_r \approx$ 1.830 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4

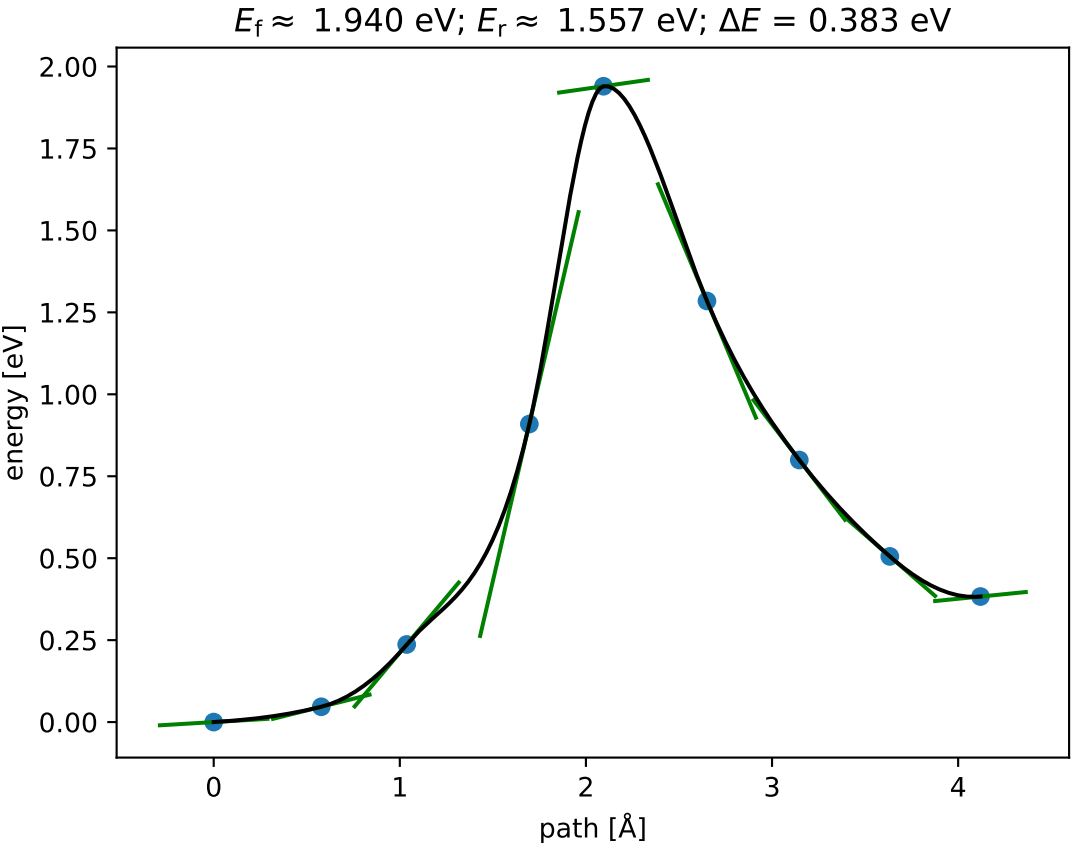

$E_f \approx$ 2.061 eV; $E_r \approx$ 1.678 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4


$E_f \approx$ 2.050 eV; $E_r \approx$ 1.667 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4


$E_f \approx$ 2.028 eV; $E_r \approx$ 1.645 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4


$E_f \approx$ 1.993 eV; $E_r \approx$ 1.610 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
0
1
2
3
4


$E_f \approx$ 1.942 eV; $E_r \approx$ 1.559 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4


$E_f \approx$ 1.940 eV; $E_r \approx$ 1.557 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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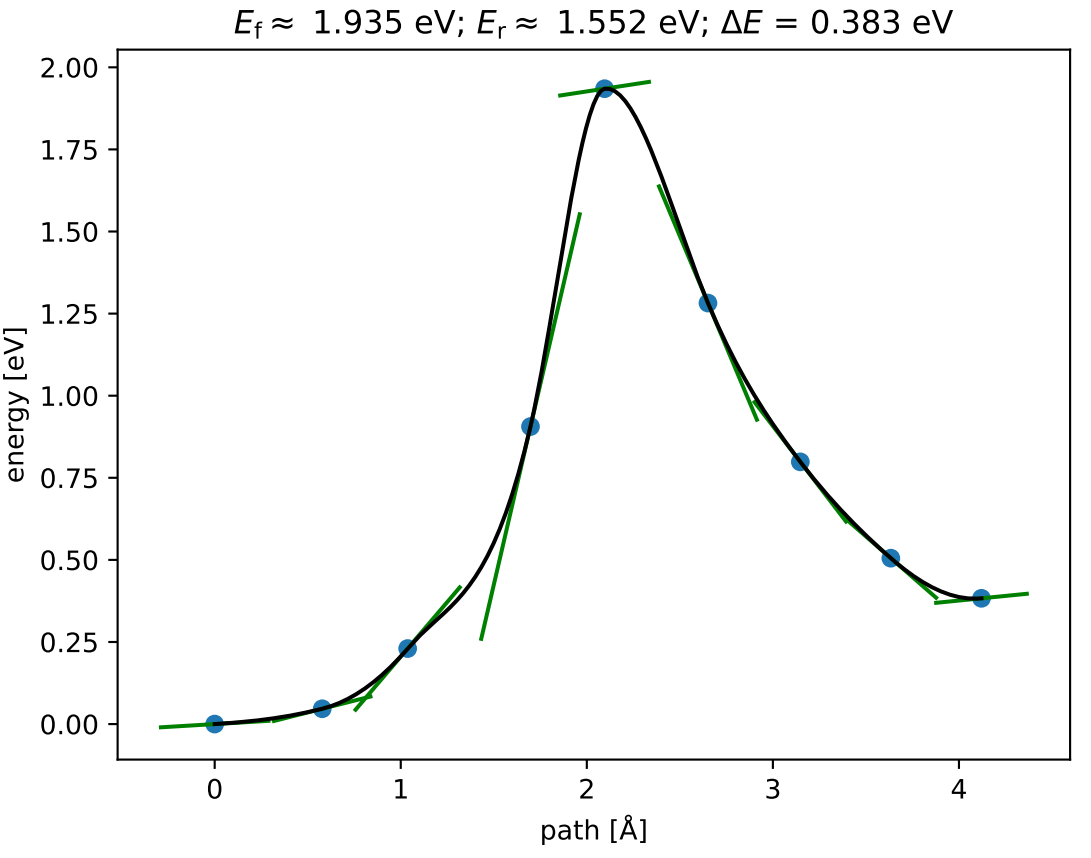
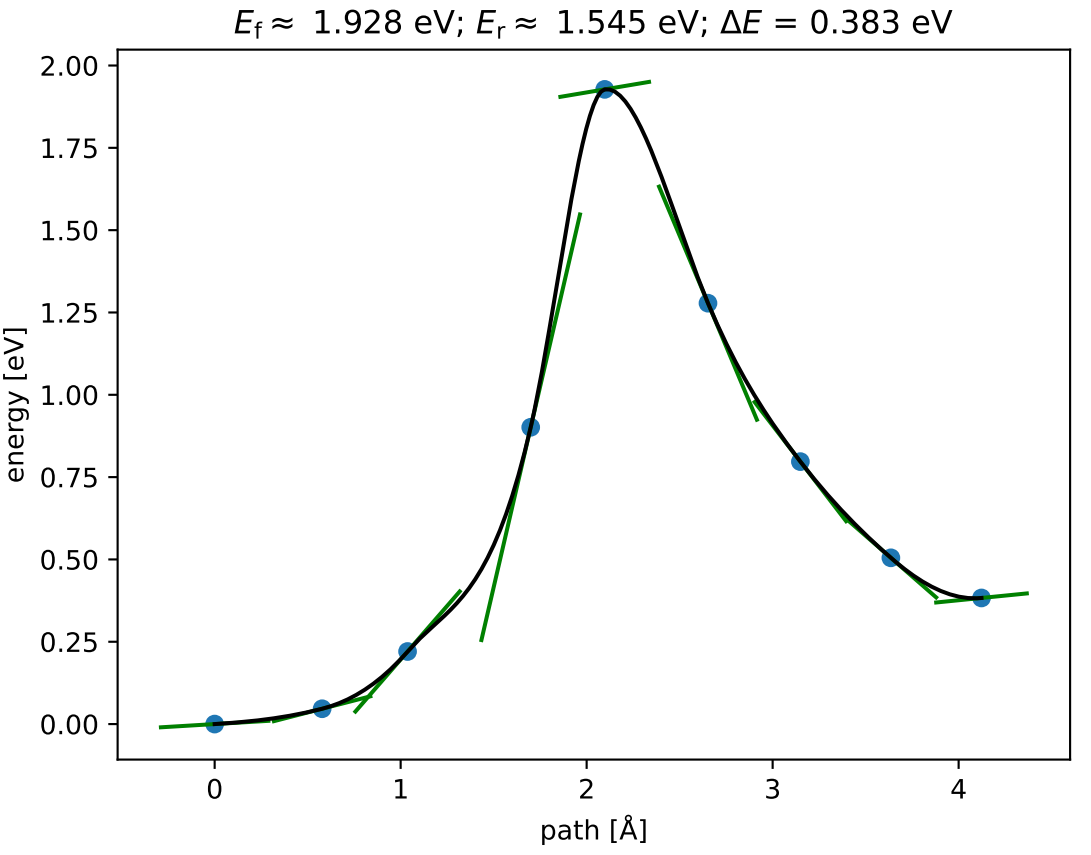
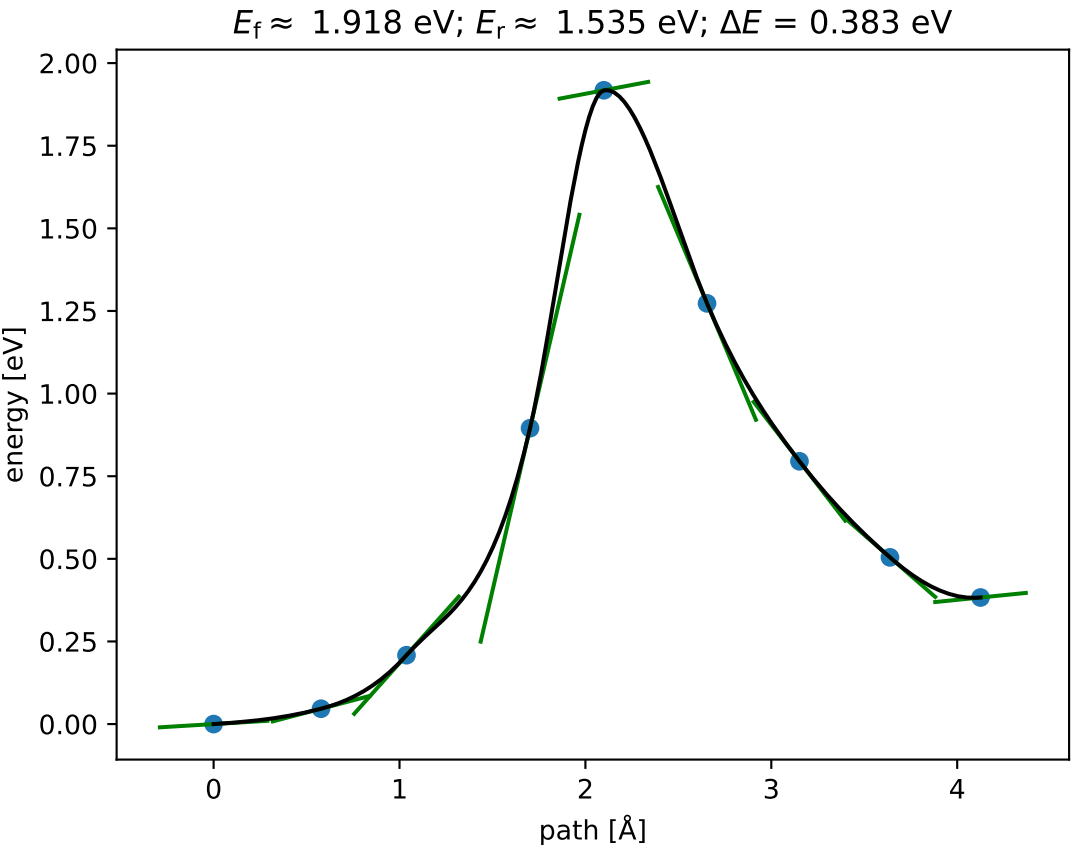
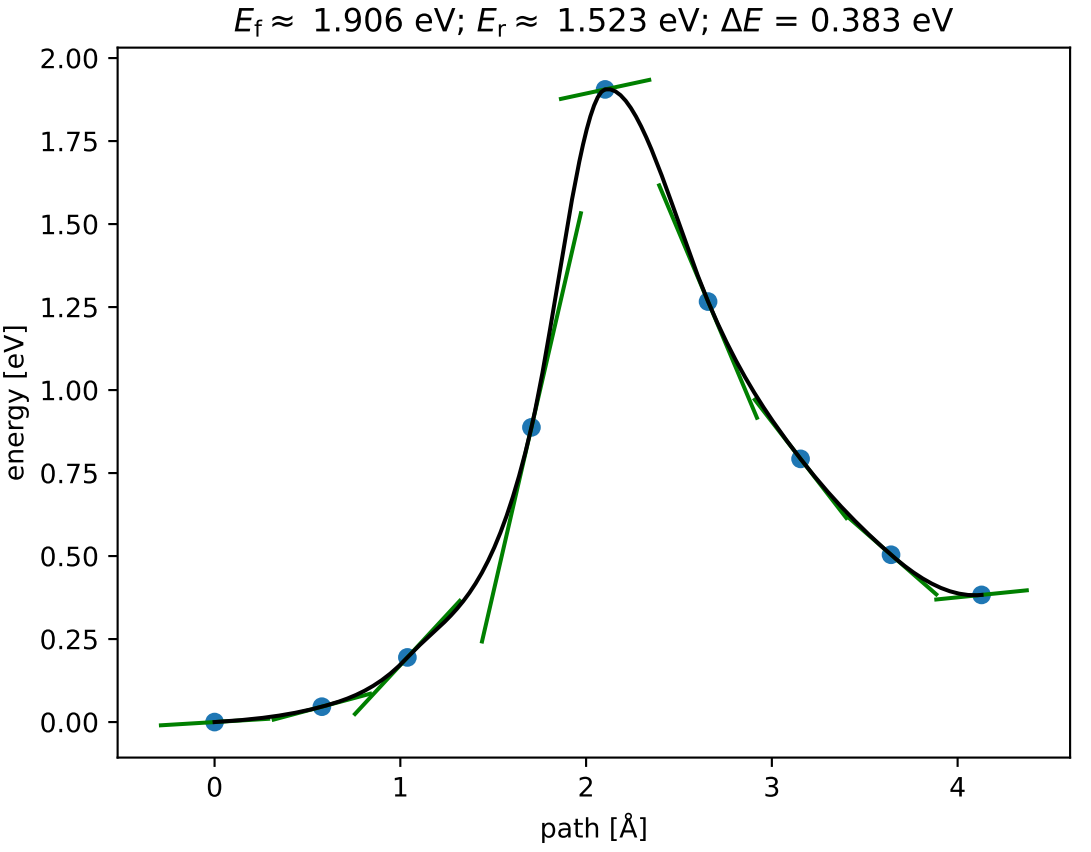
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
0
1
2
3
4


$E_f \approx$ 1.935 eV; $E_r \approx$ 1.552 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4


$E_f \approx$ 1.928 eV; $E_r \approx$ 1.545 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4


$E_f \approx$ 1.918 eV; $E_r \approx$ 1.535 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
0
1
2
3
4


$E_f \approx$ 1.906 eV; $E_r \approx$ 1.523 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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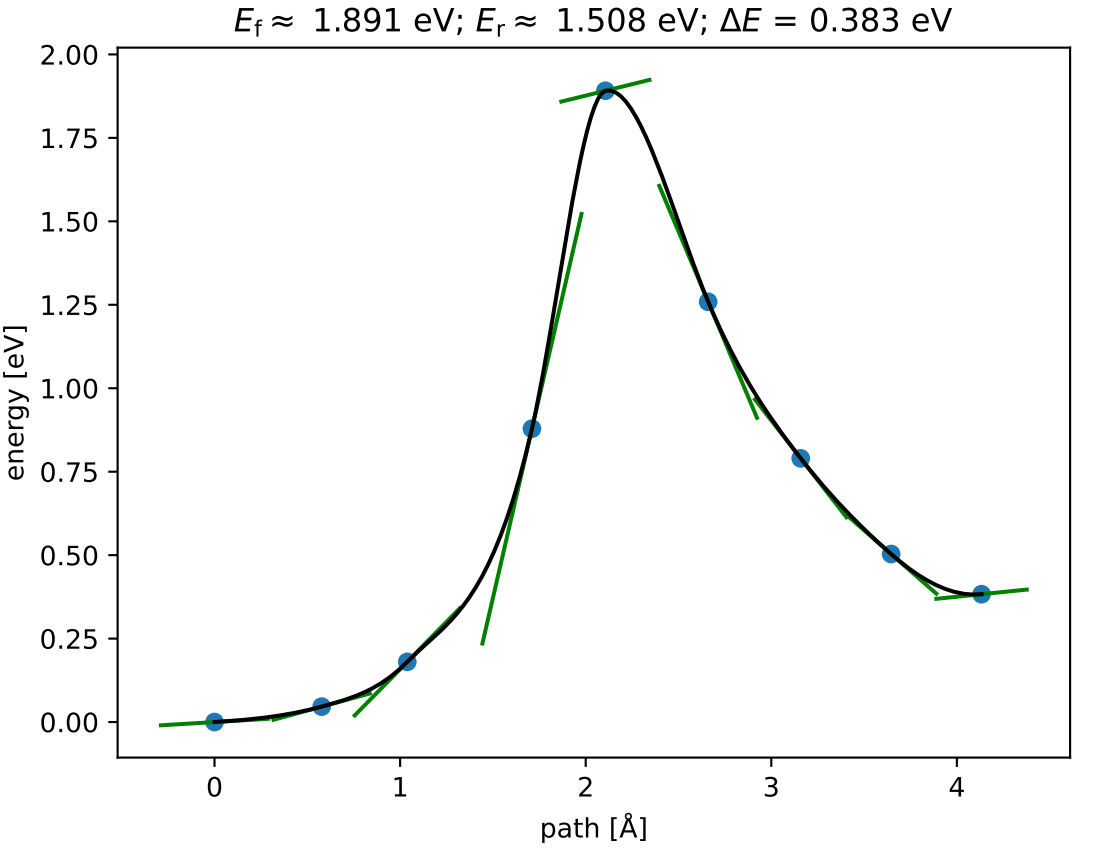
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4


$E_f \approx$ 1.891 eV; $E_r \approx$ 1.508 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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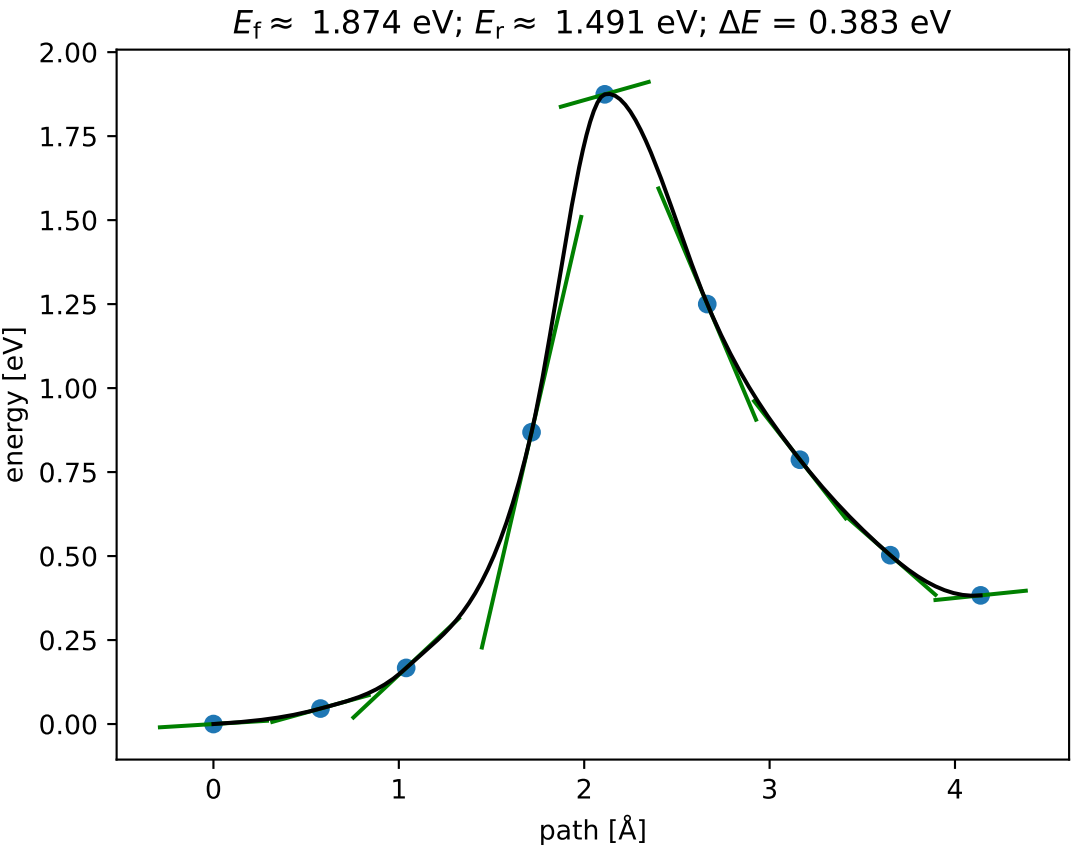
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4


$E_f \approx$ 1.874 eV; $E_r \approx$ 1.491 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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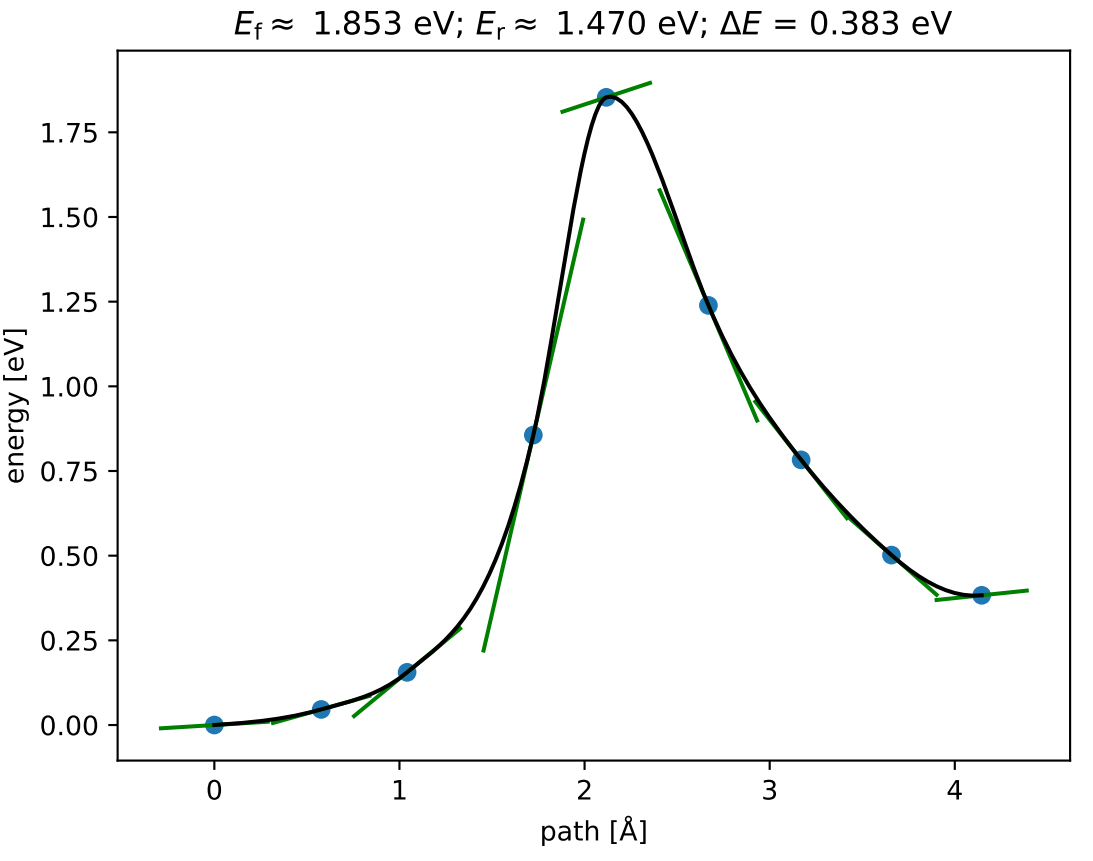
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4


$E_f \approx$ 1.853 eV; $E_r \approx$ 1.470 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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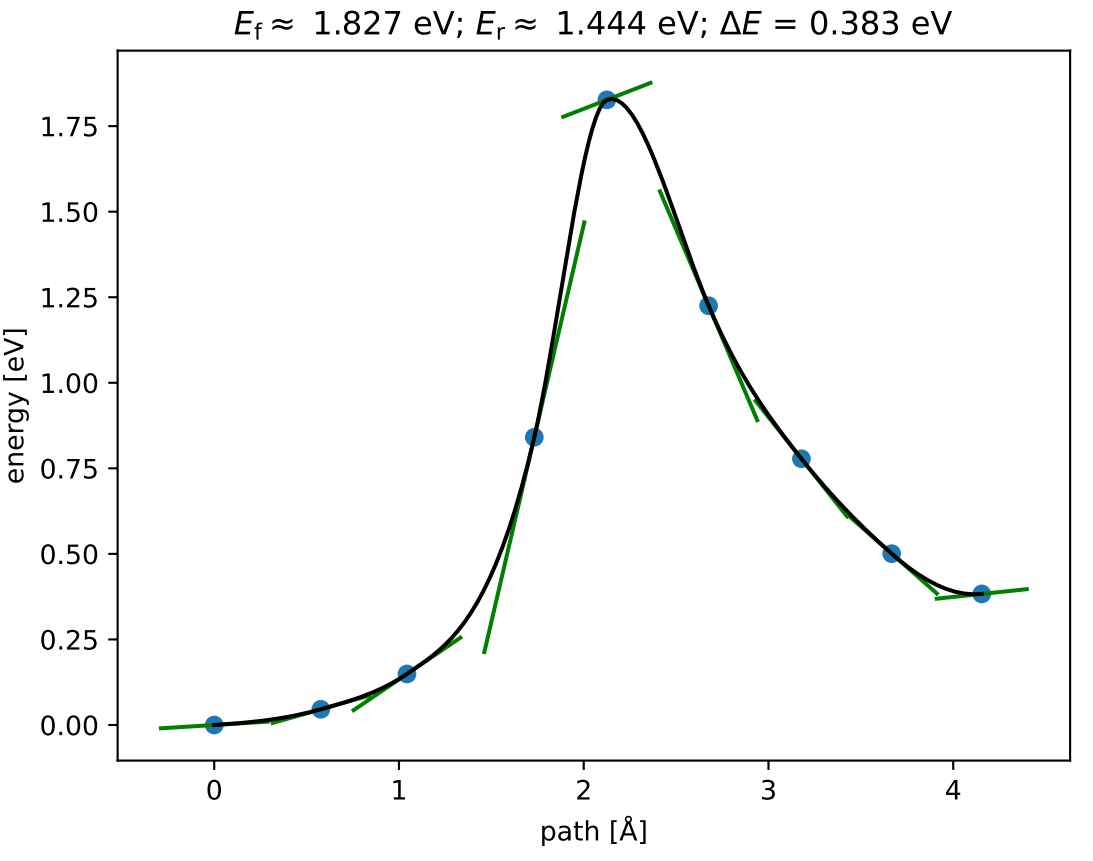
0.25
0.50
0.75
1.00
1.25
1.50
1.75
0
1
2
3
4


$E_f \approx$ 1.827 eV; $E_r \approx$ 1.444 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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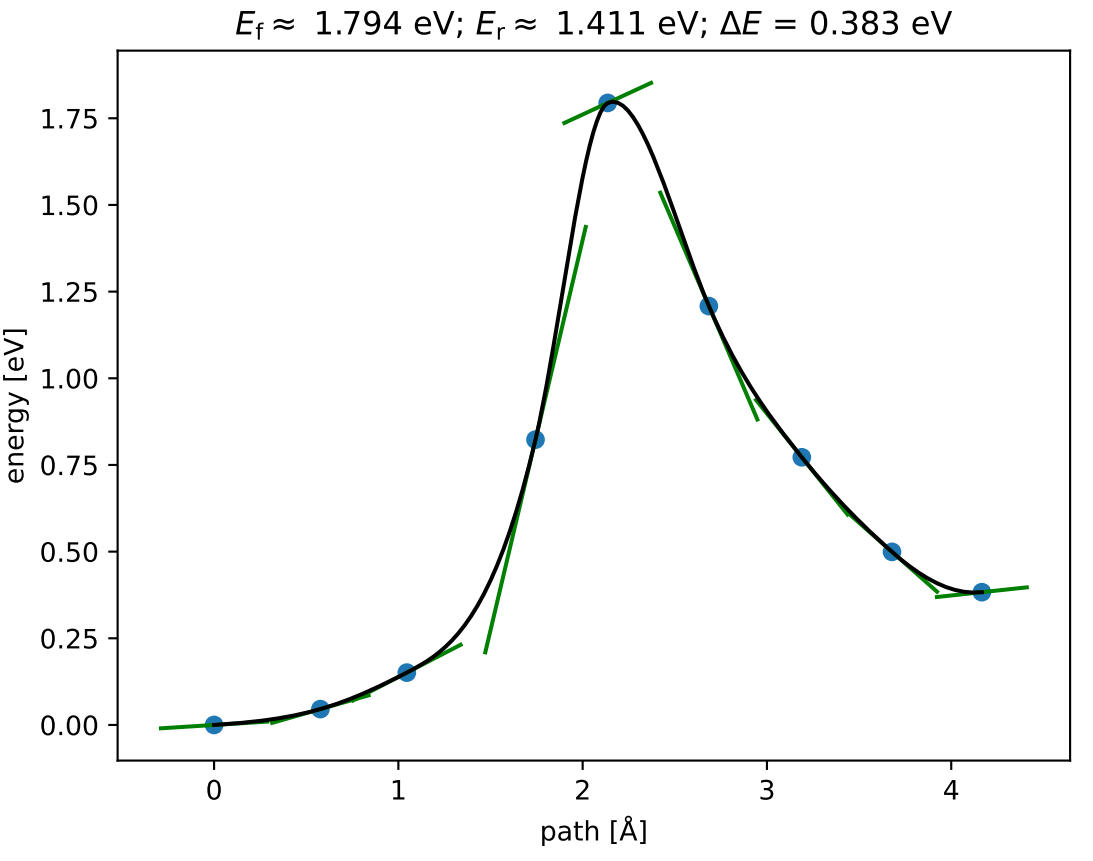
0.25
0.50
0.75
1.00
1.25
1.50
1.75
0
1
2
3
4


$E_f \approx$ 1.794 eV; $E_r \approx$ 1.411 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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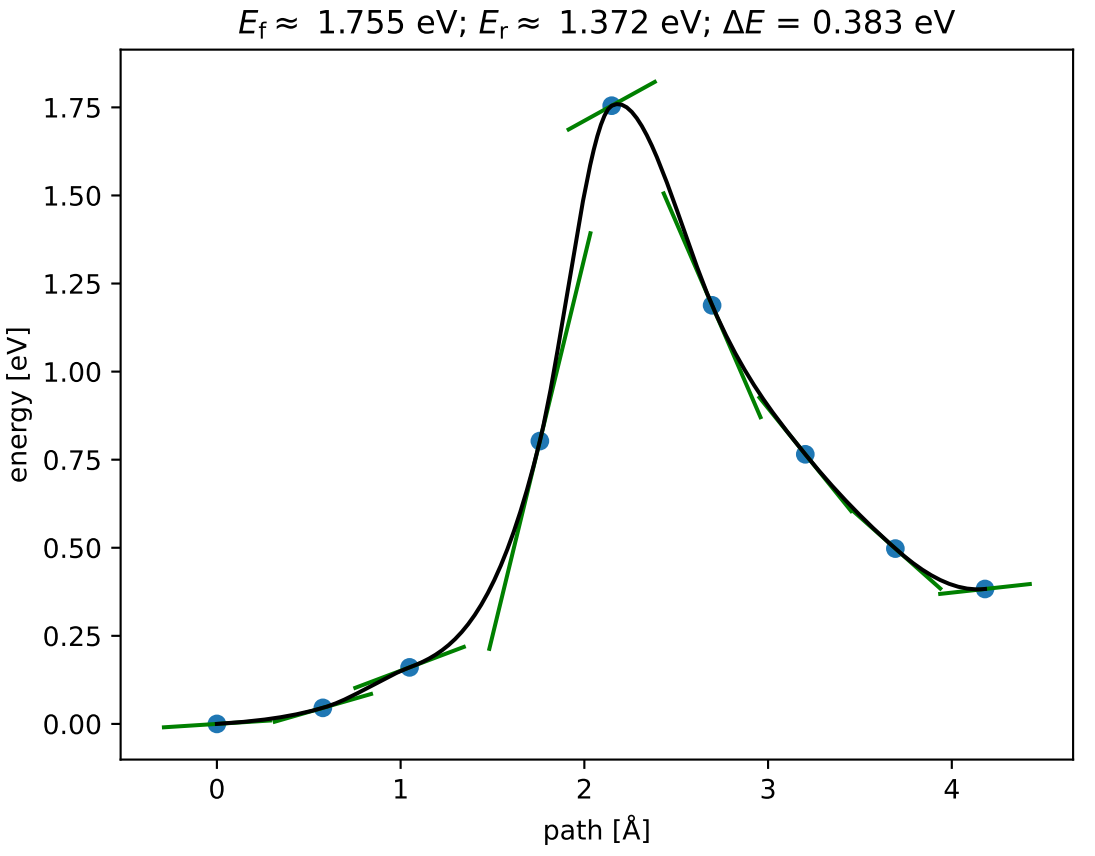
0.50
0.75
1.00
1.25
1.50
1.75
0
1
2
3
4


$E_f \approx$ 1.755 eV; $E_r \approx$ 1.372 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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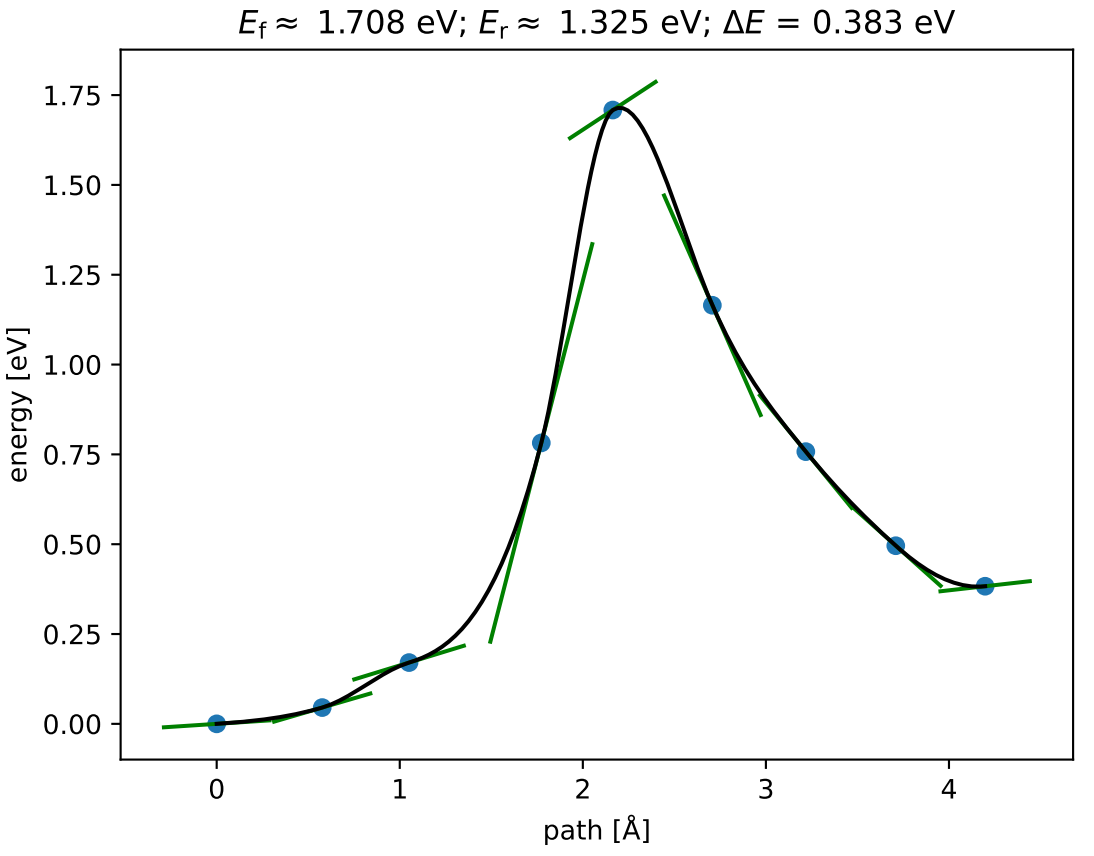
0.25
0.50
0.75
1.00
1.25
1.50
1.75
0
1
2
3
4


$E_f \approx$ 1.708 eV; $E_r \approx$ 1.325 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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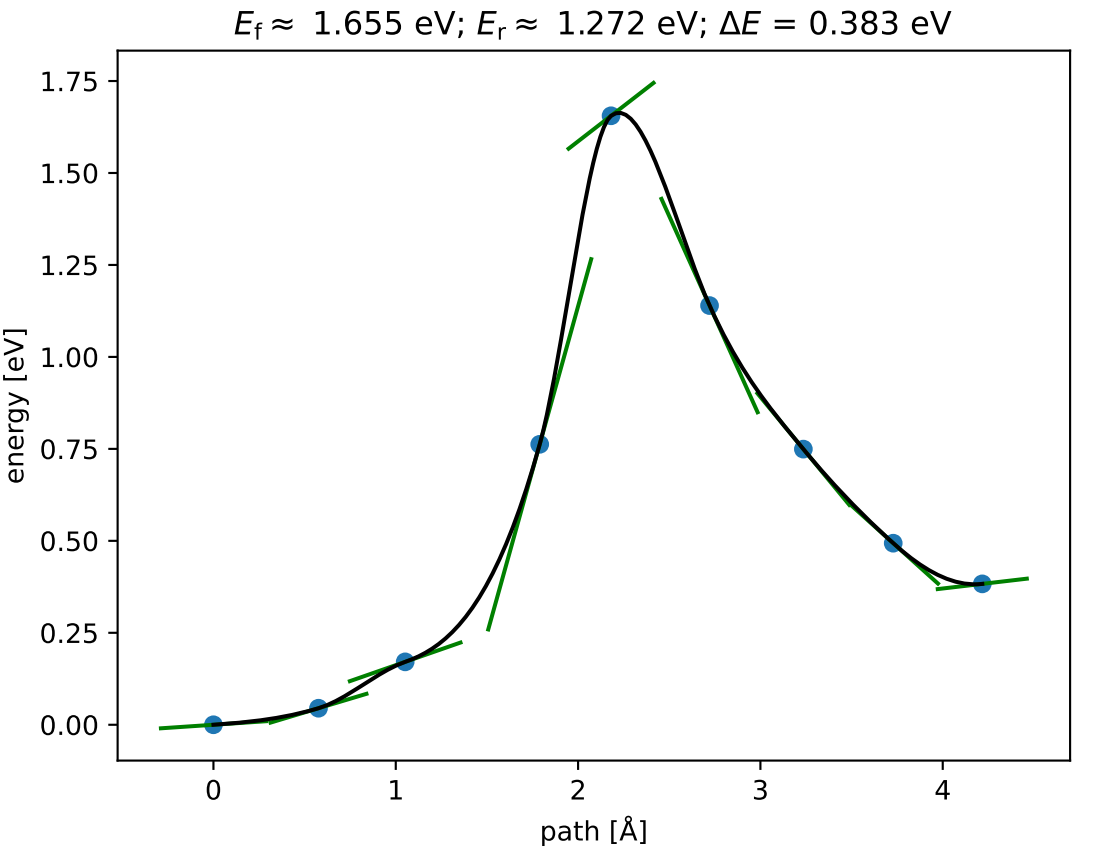
0.25
0.50
0.75
1.00
1.25
1.50
1.75
0
1
2
3
4


$E_f \approx$ 1.655 eV; $E_r \approx$ 1.272 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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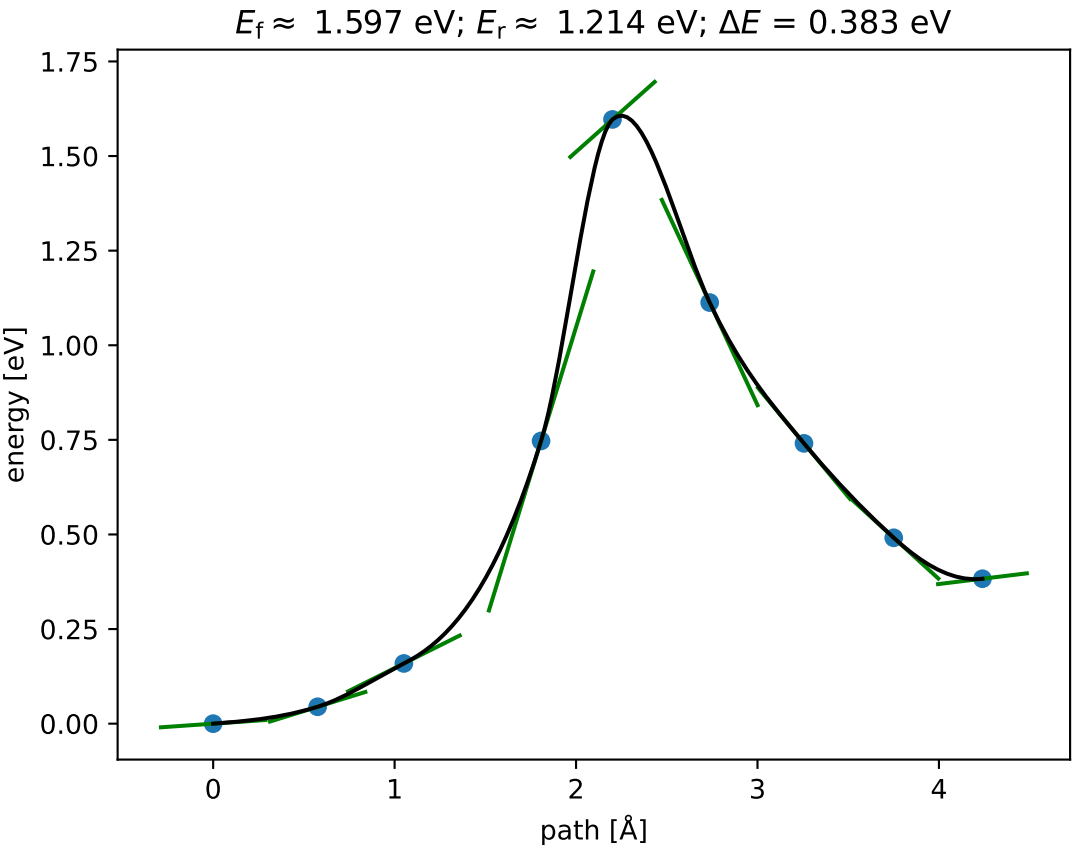
0.25
0.50
0.75
1.00
1.25
1.50
1.75
0
1
2
3
4


$E_f \approx$ 1.597 eV; $E_r \approx$ 1.214 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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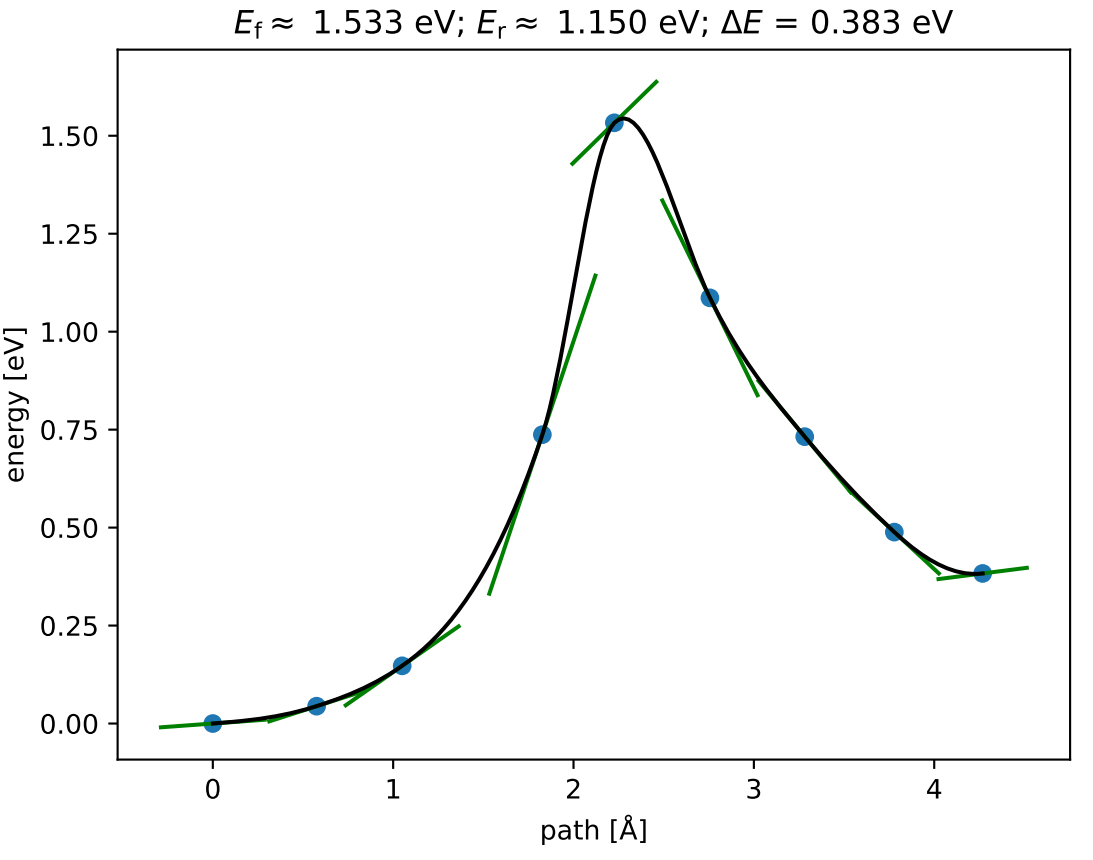
0.25
0.50
0.75
1.00
1.25
1.50
1.75
0
1
2
3
4


$E_f \approx$ 1.533 eV; $E_r \approx$ 1.150 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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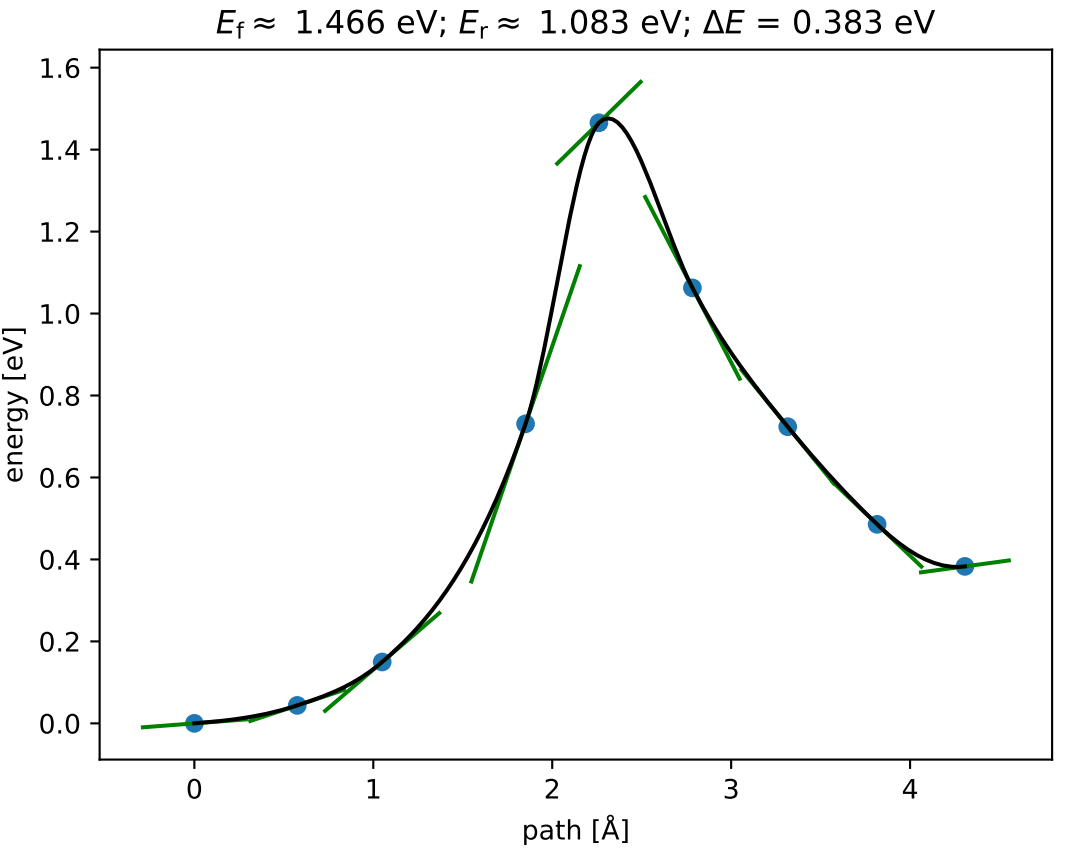
0.25
0.50
0.75
1.00
1.25
1.50
0
1
2
3
4


$E_f \approx$ 1.466 eV; $E_r \approx$ 1.083 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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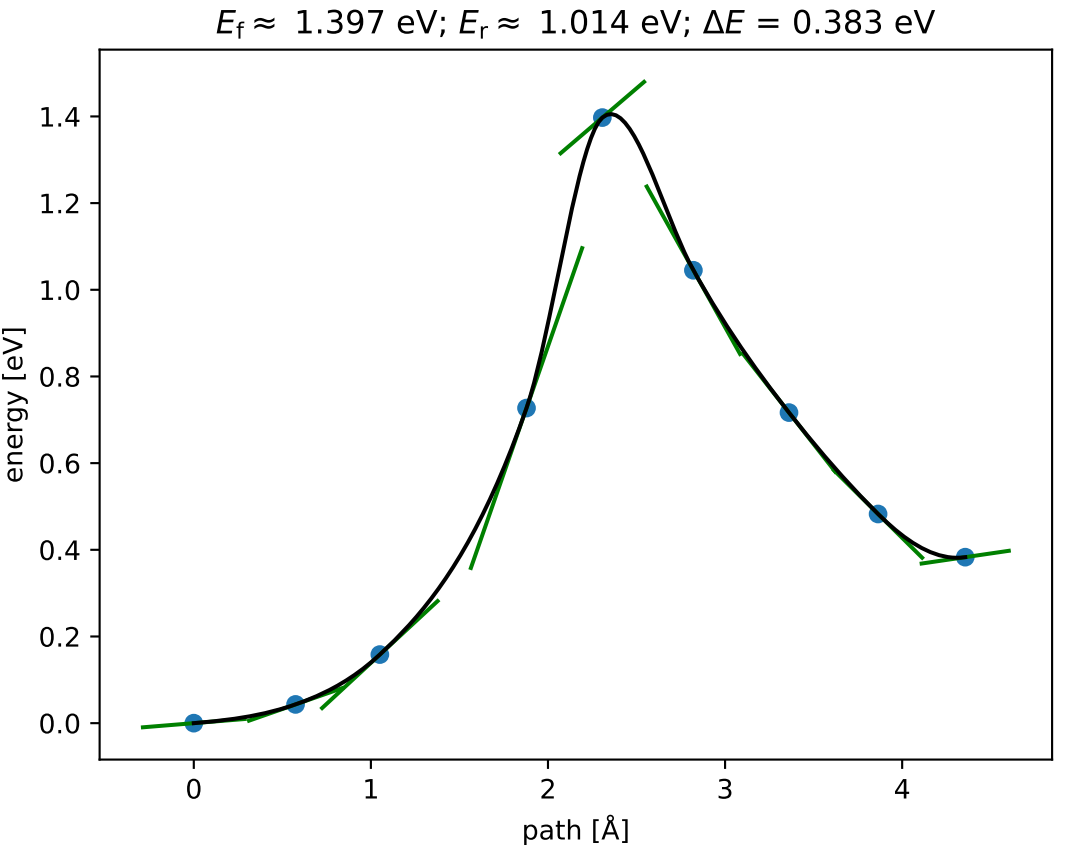
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
1
2
3
4


$E_f \approx$ 1.397 eV; $E_r \approx$ 1.014 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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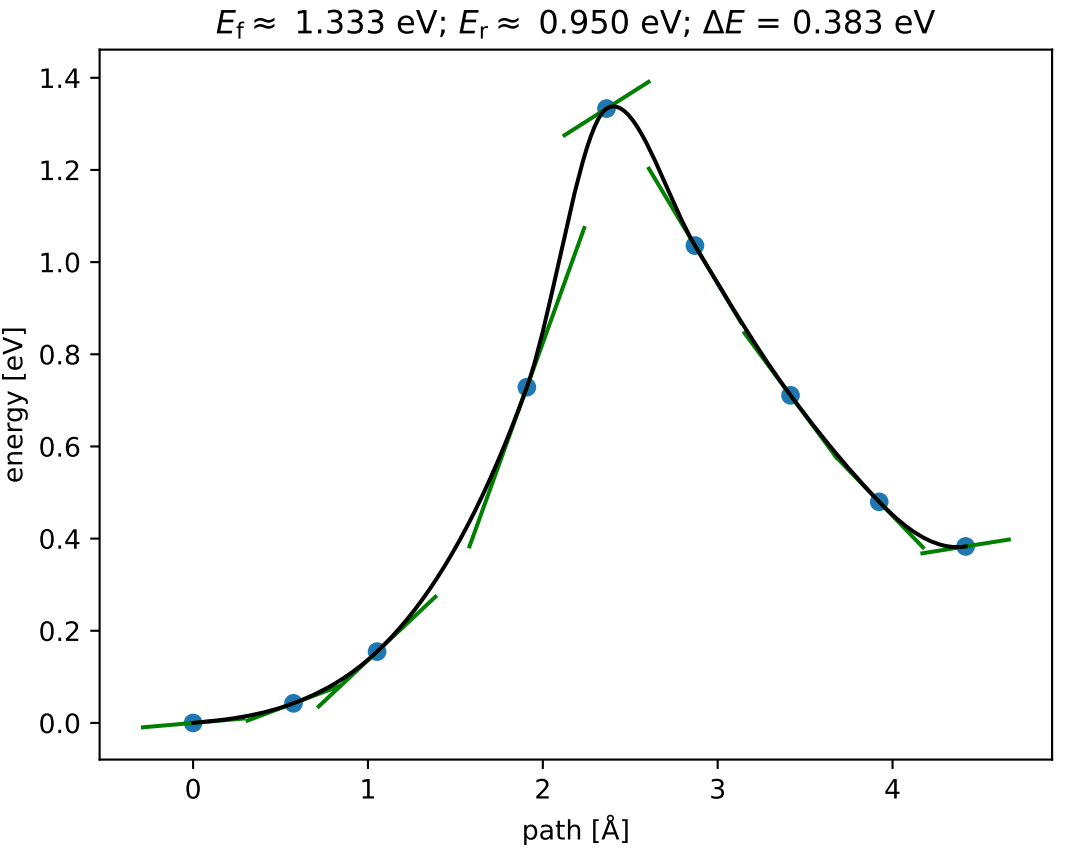
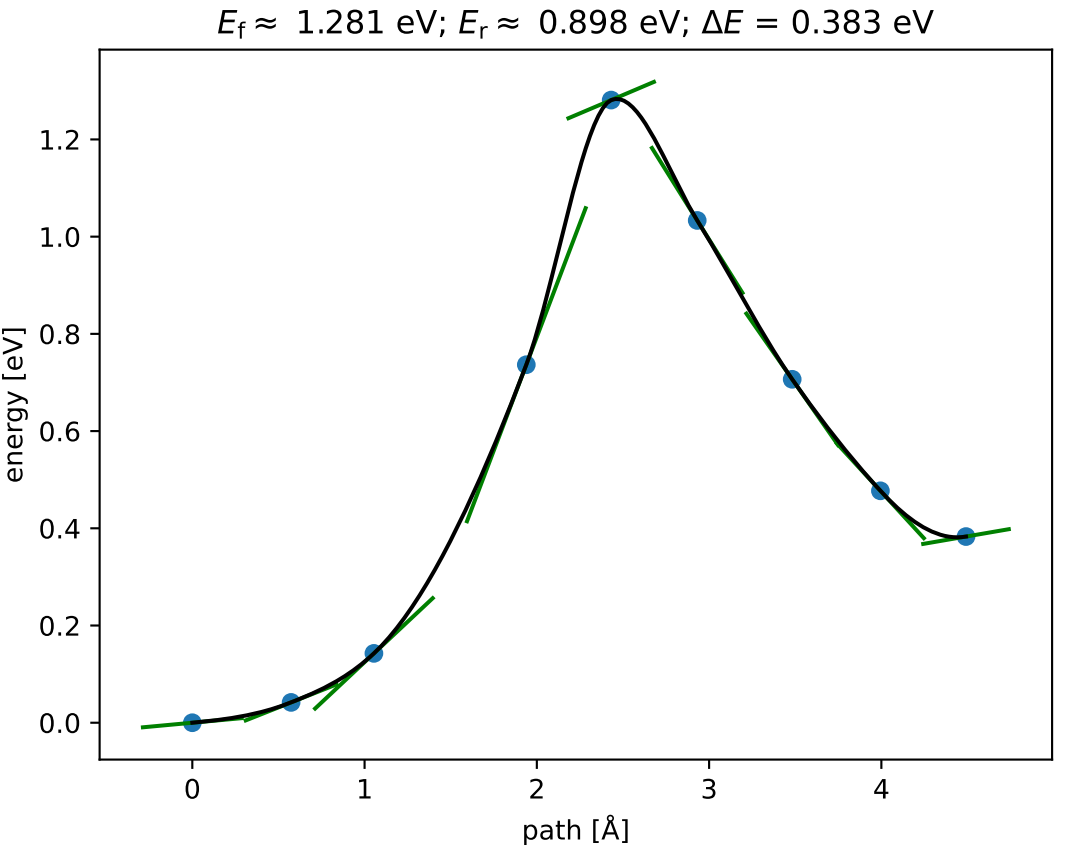
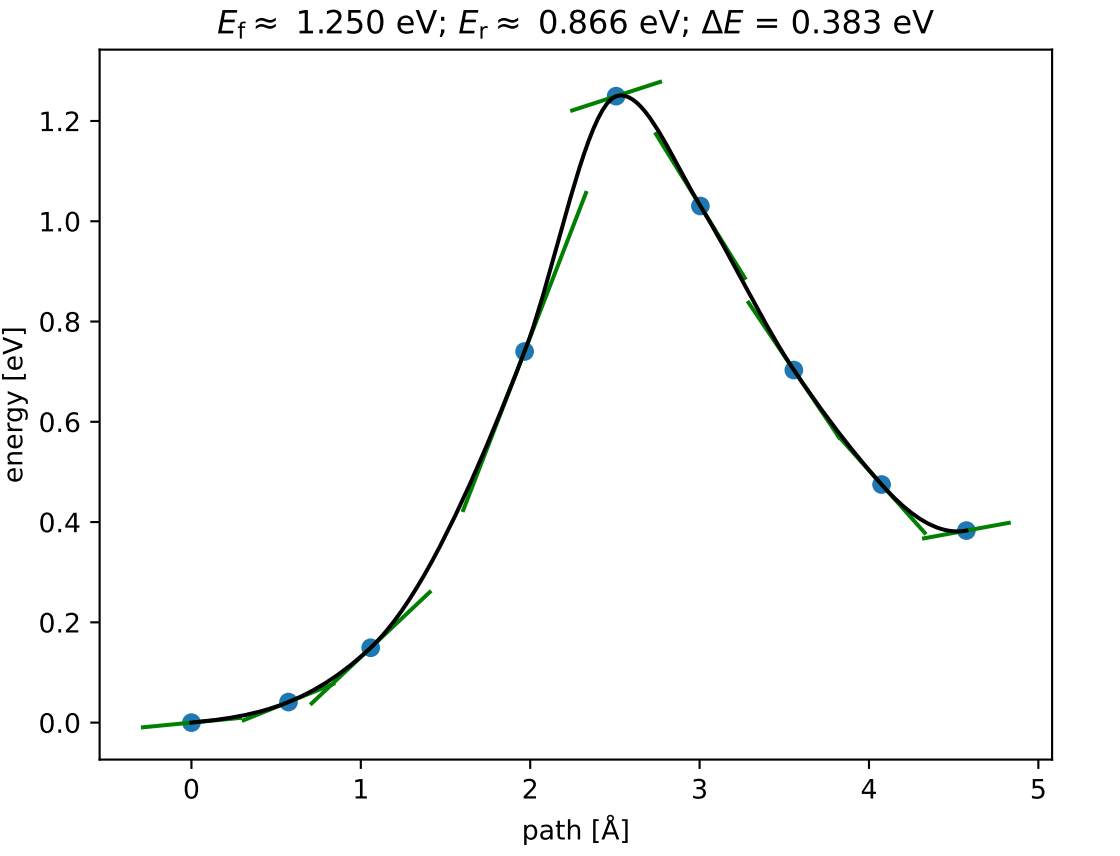
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4


$E_f \approx$ 1.333 eV; $E_r \approx$ 0.950 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4


$E_f \approx$ 1.281 eV; $E_r \approx$ 0.898 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4


$E_f \approx$ 1.250 eV; $E_r \approx$ 0.866 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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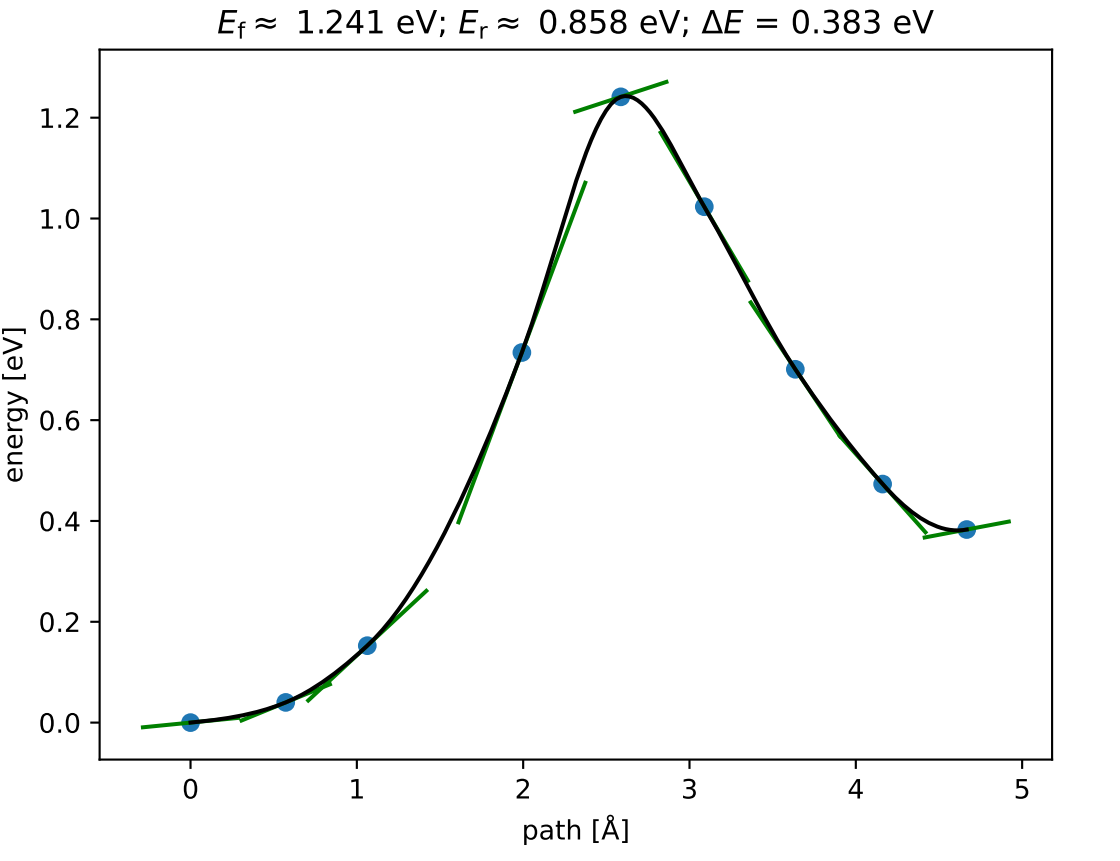
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.241 eV; $E_r \approx$ 0.858 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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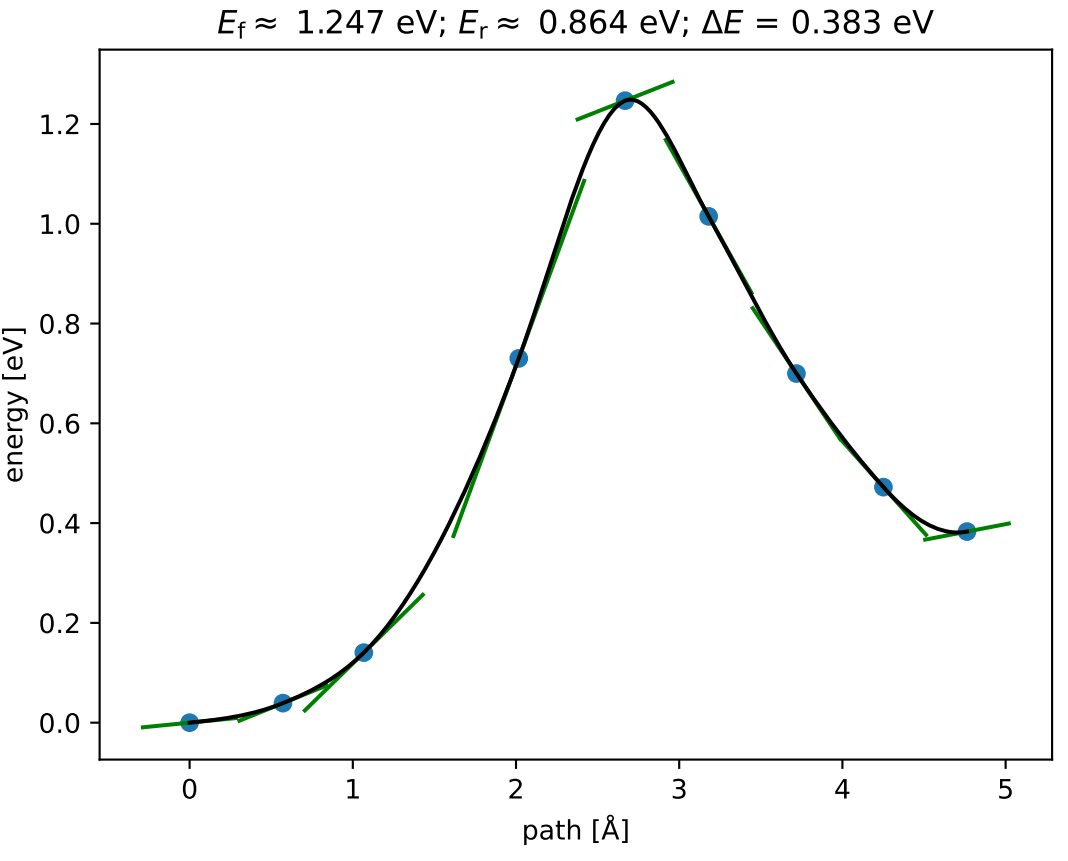
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.247 eV; $E_r \approx$ 0.864 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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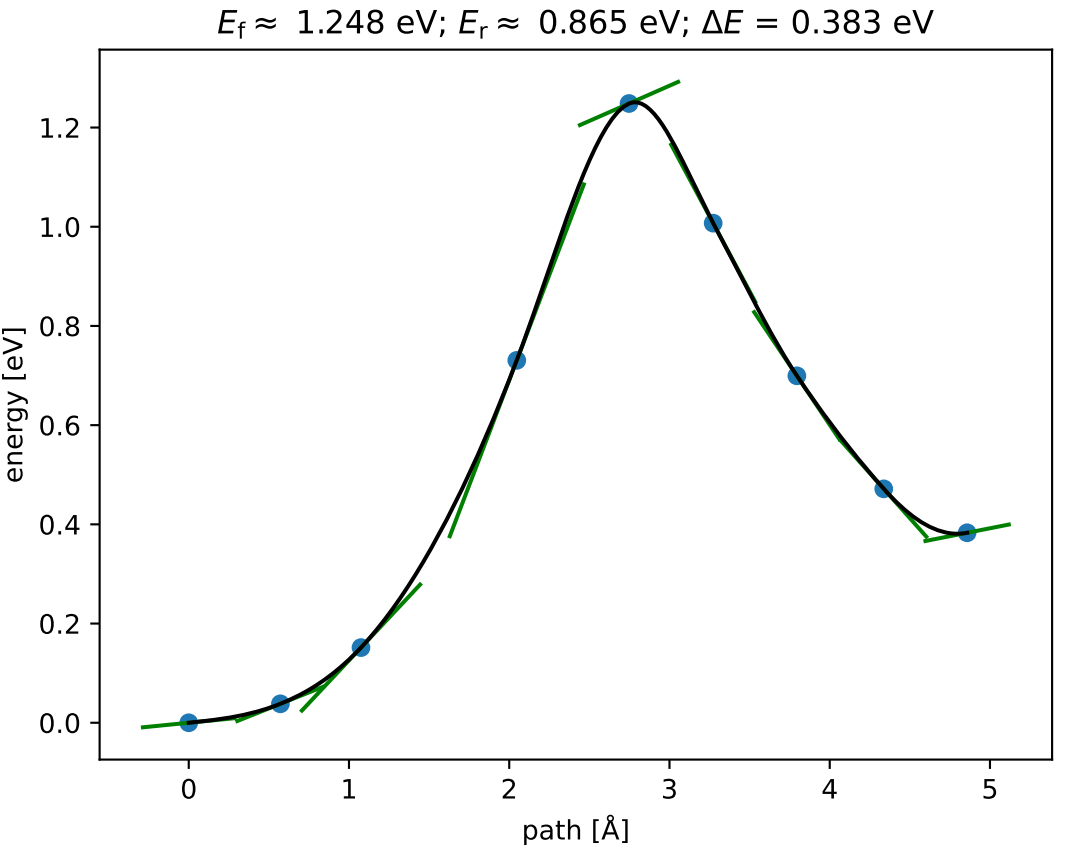
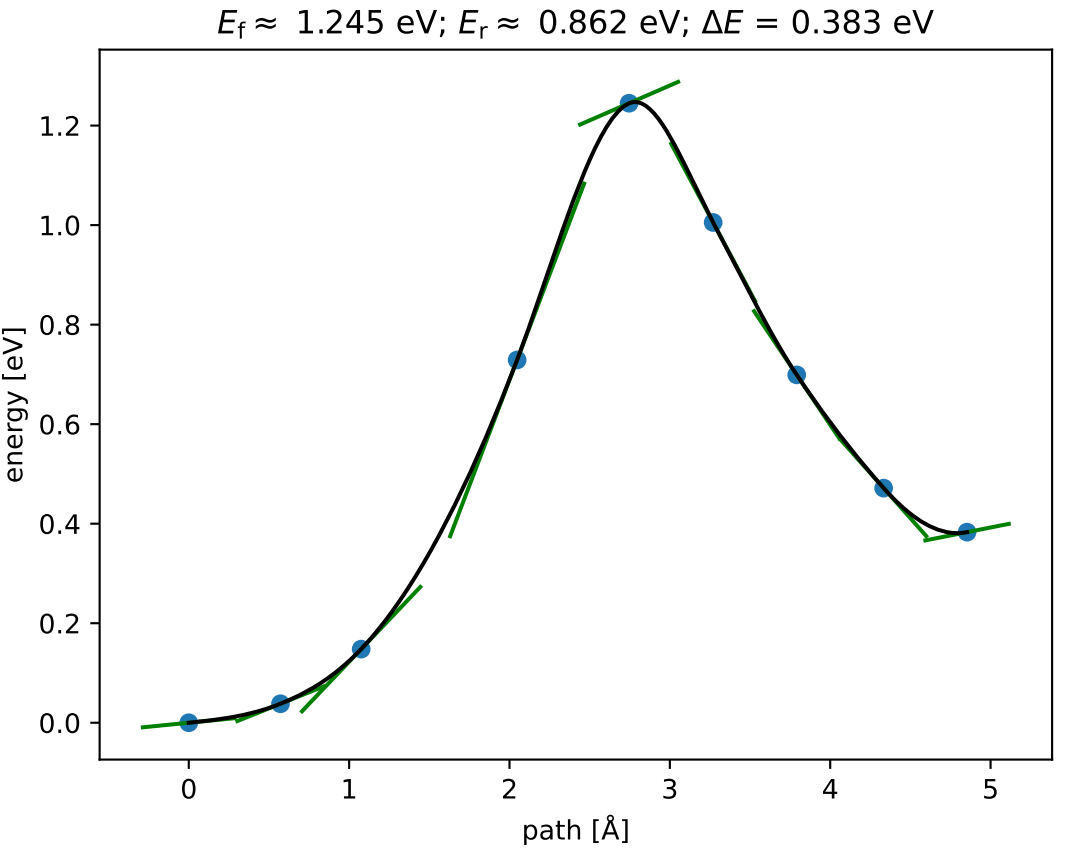
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.248 eV; $E_r \approx$ 0.865 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.245 eV; $E_r \approx$ 0.862 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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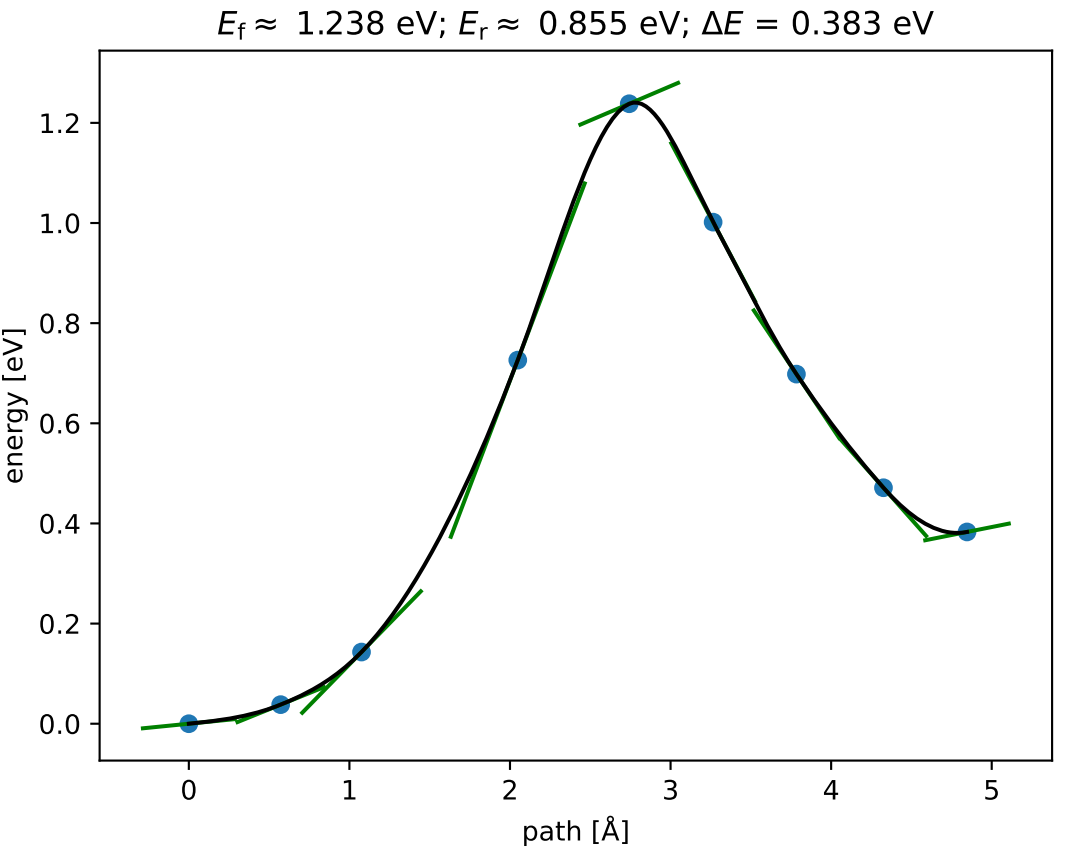
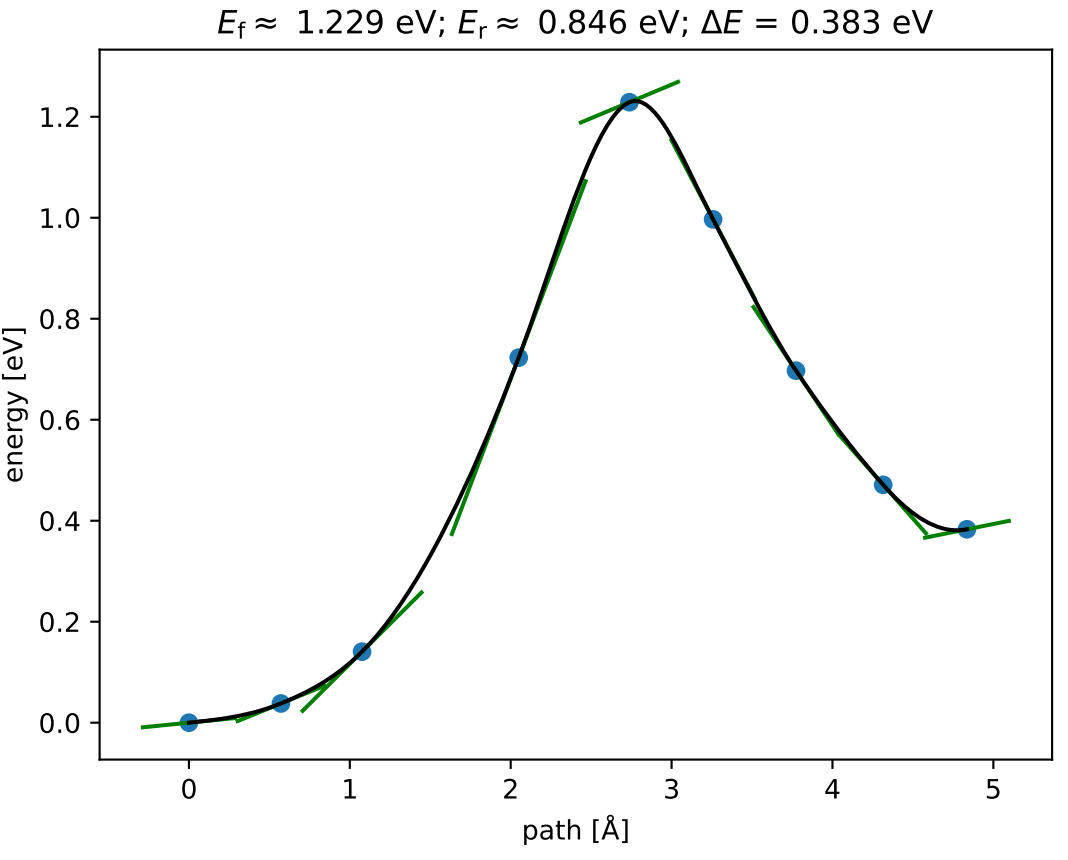
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.238 eV; $E_r \approx$ 0.855 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.229 eV; $E_r \approx$ 0.846 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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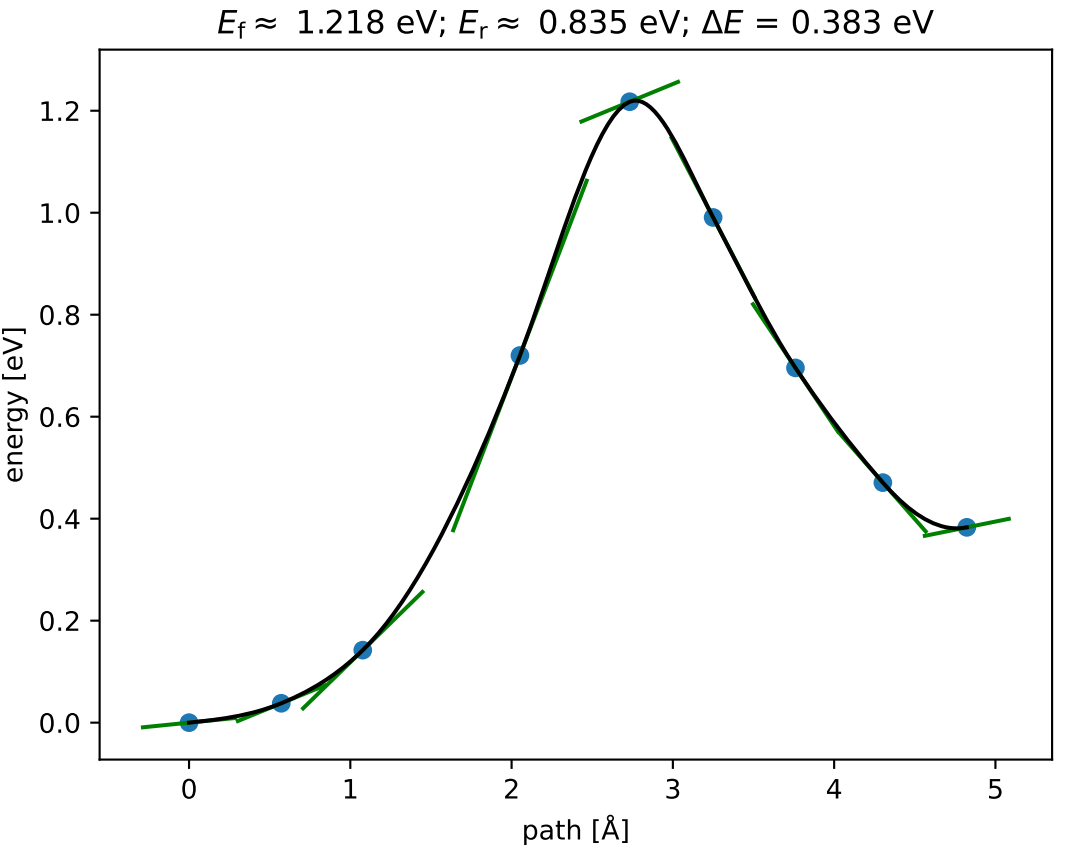
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.218 eV; $E_r \approx$ 0.835 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.8
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1.2
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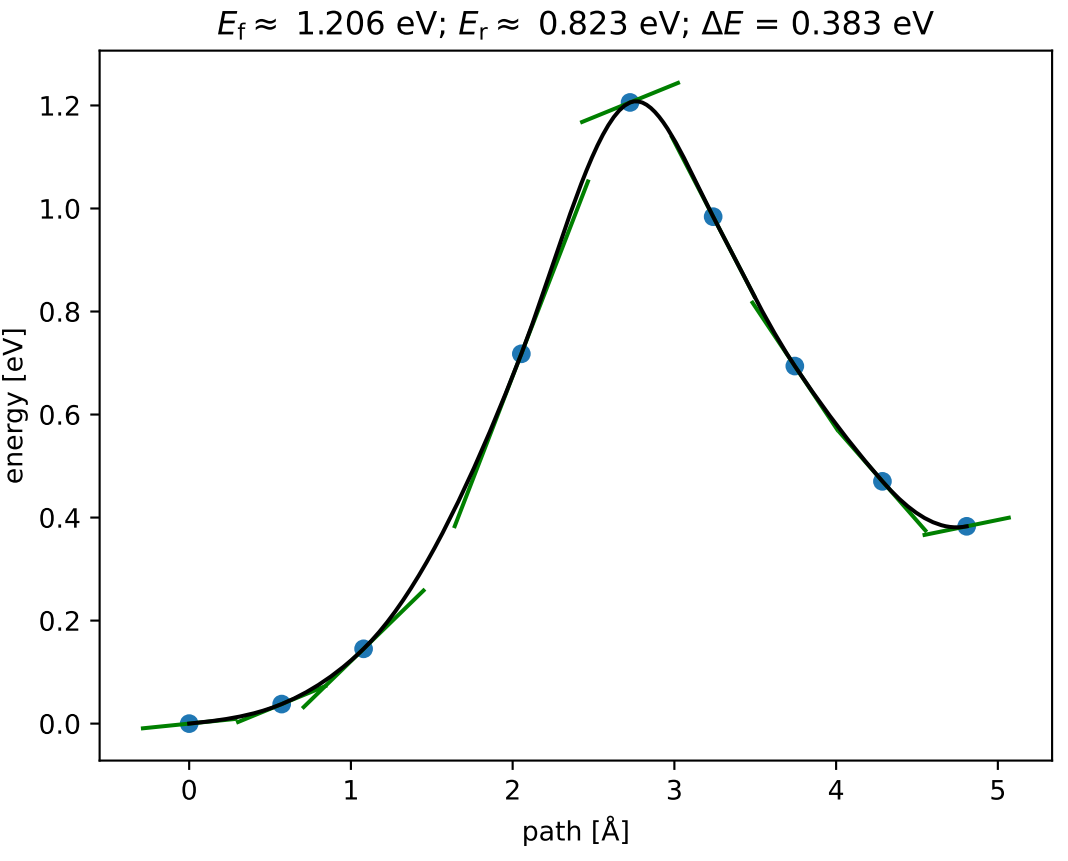
2
3
4
5


$E_f \approx$ 1.206 eV; $E_r \approx$ 0.823 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.6
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1.2
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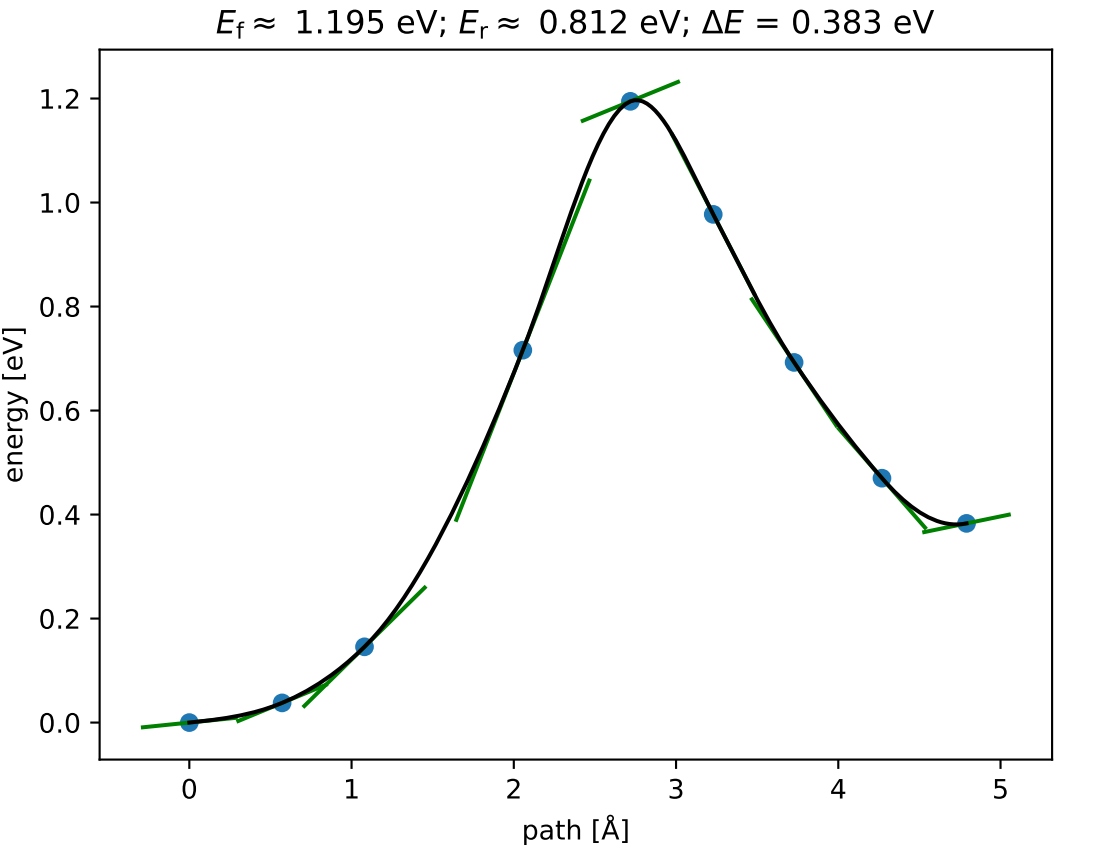
3
4
5


$E_f \approx$ 1.195 eV; $E_r \approx$ 0.812 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.6
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4
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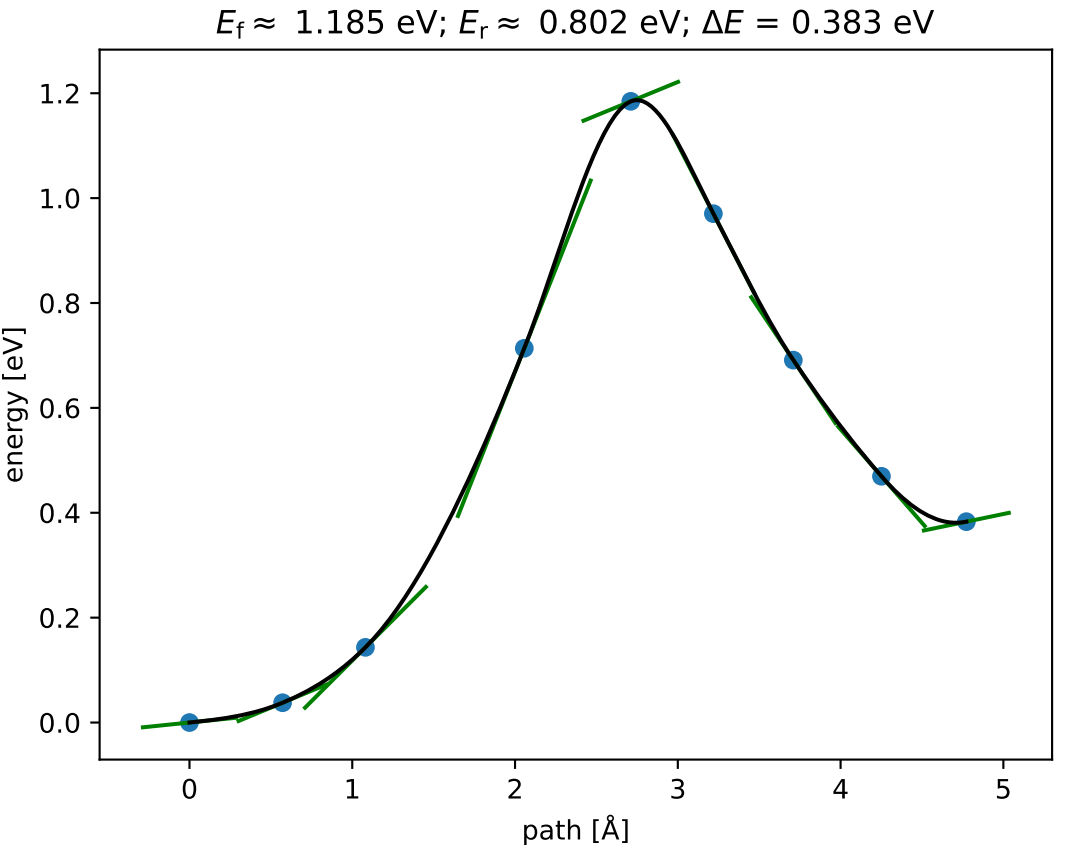
$E_f \approx$ 1.185 eV; $E_r \approx$ 0.802 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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1.2
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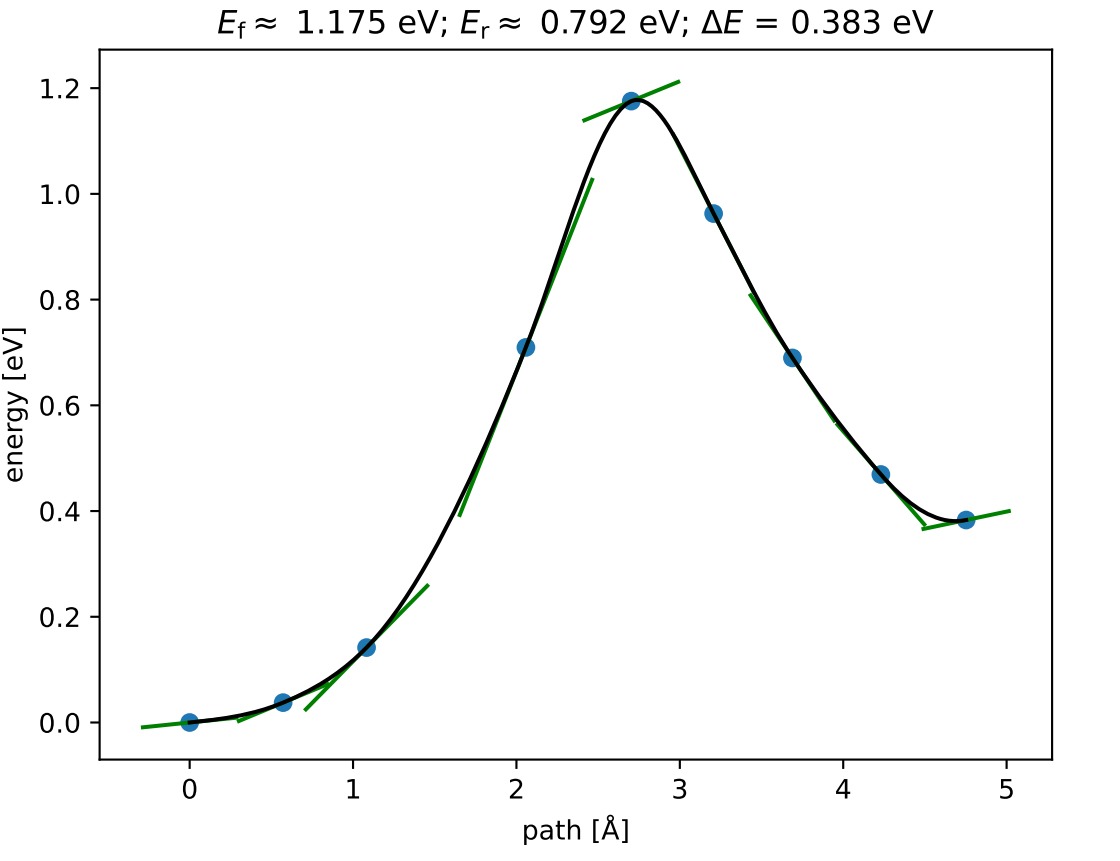
3
4
5


$E_f \approx$ 1.175 eV; $E_r \approx$ 0.792 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.8
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1.2
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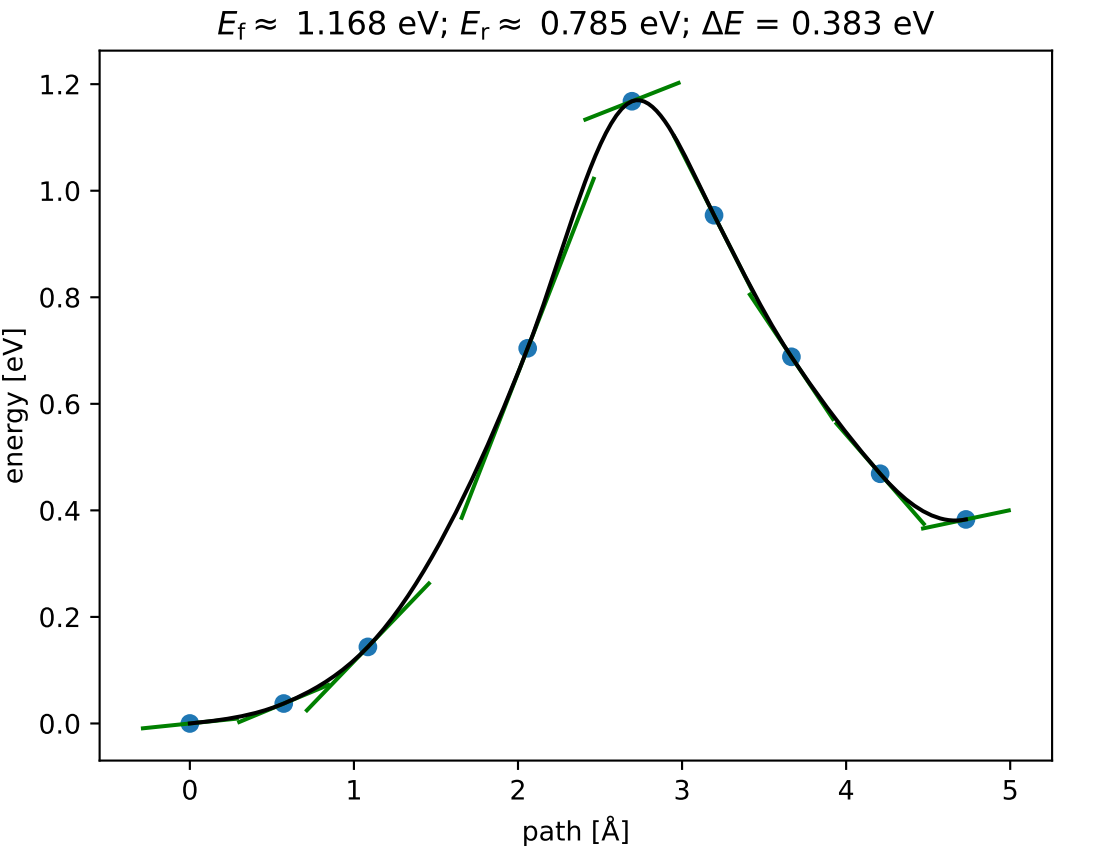
2
3
4
5


$E_f \approx$ 1.168 eV; $E_r \approx$ 0.785 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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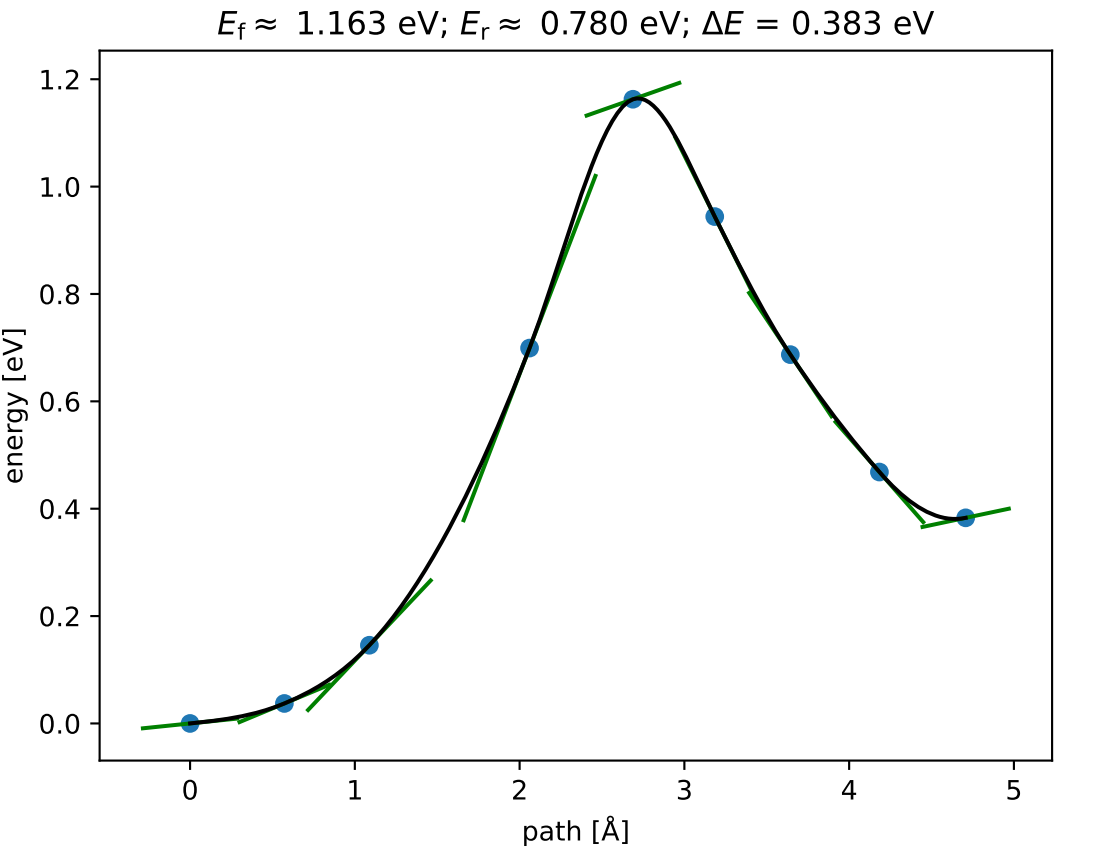
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.163 eV; $E_r \approx$ 0.780 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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1.2
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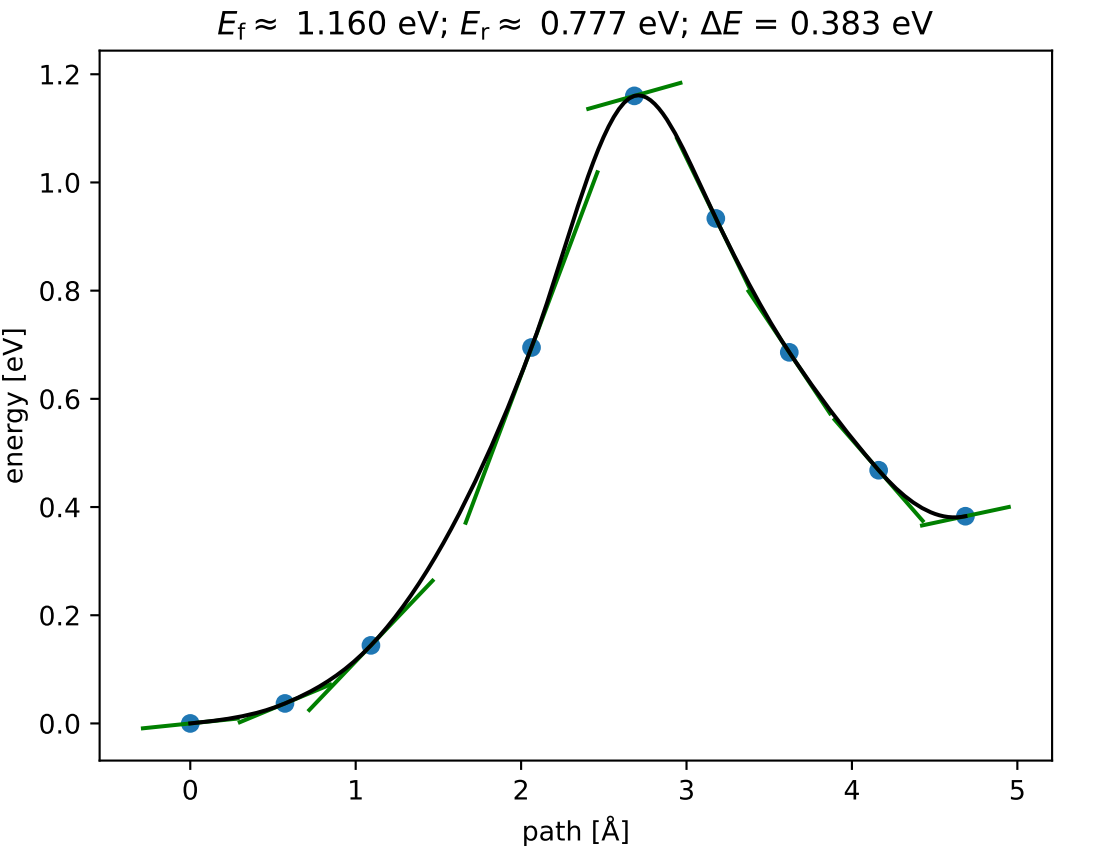
2
3
4
5


$E_f \approx$ 1.160 eV; $E_r \approx$ 0.777 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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1.2
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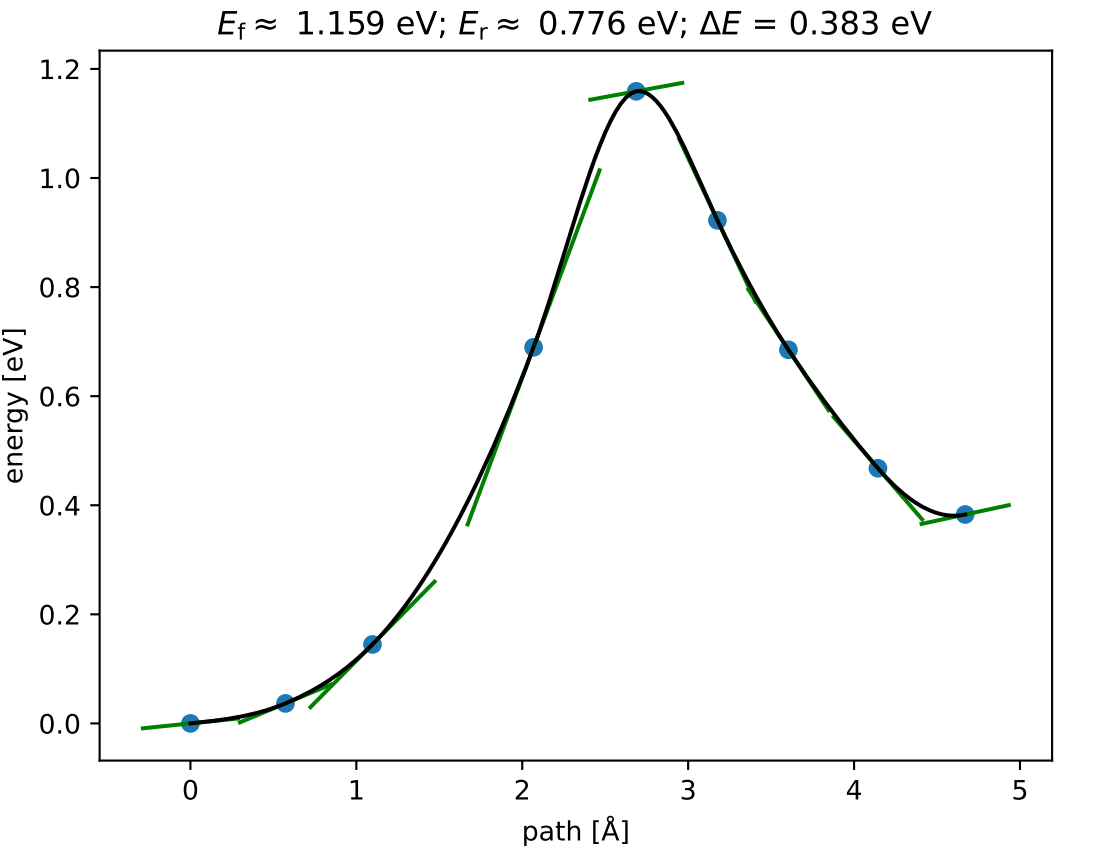
2
3
4
5


$E_f \approx$ 1.159 eV; $E_r \approx$ 0.776 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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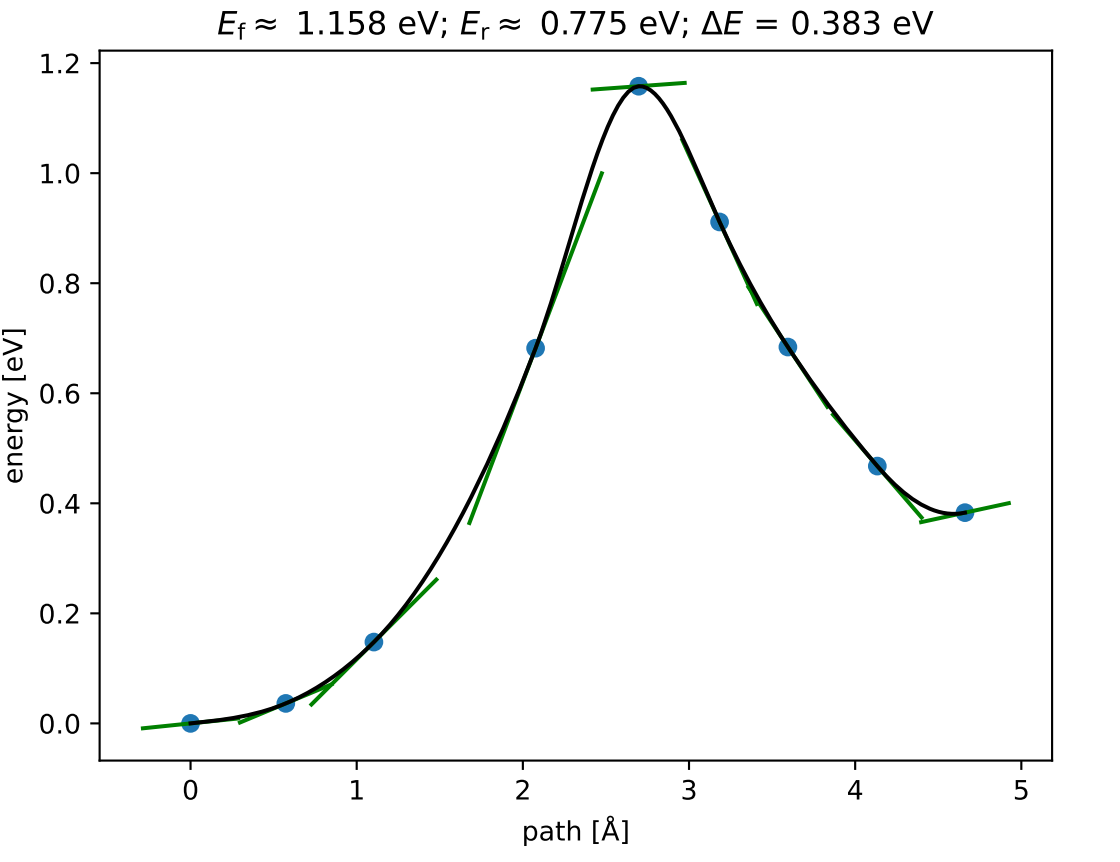
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.158 eV; $E_r \approx$ 0.775 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.6
0.8
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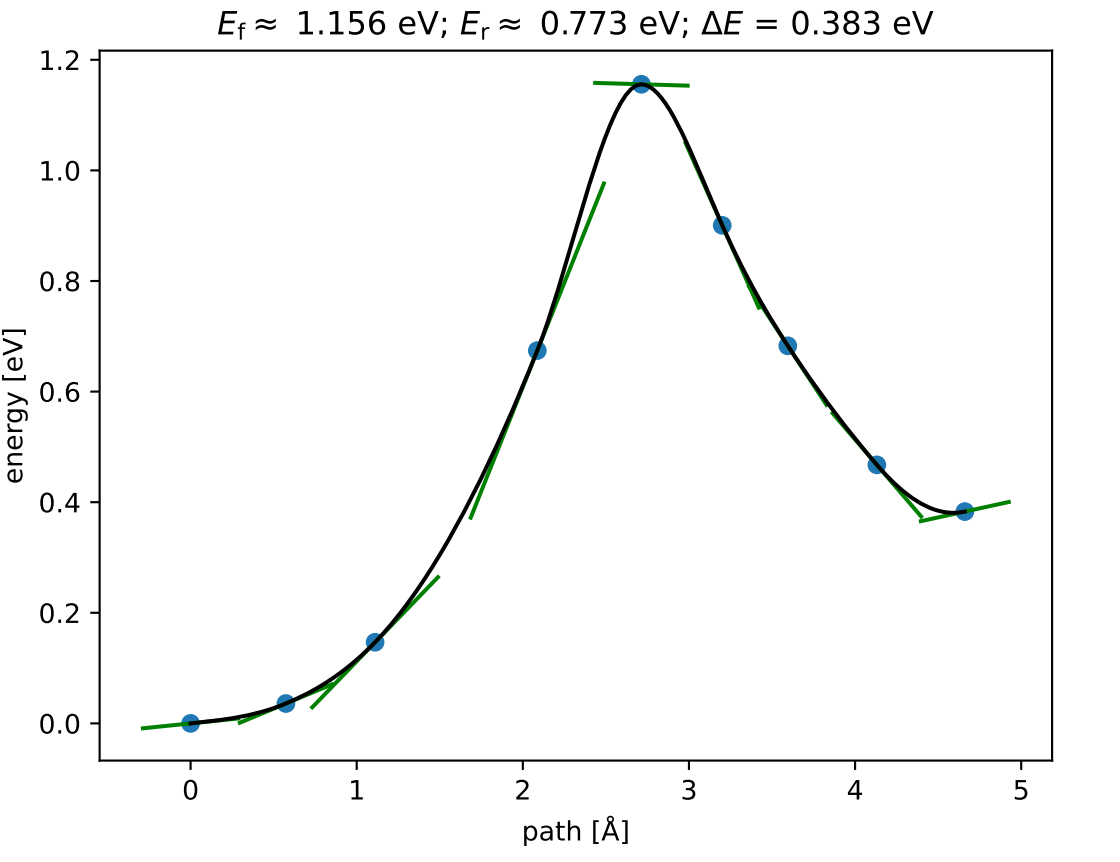
1.2
0
1
2
3
4
5


$E_f \approx$ 1.156 eV; $E_r \approx$ 0.773 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.8
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1.2
0
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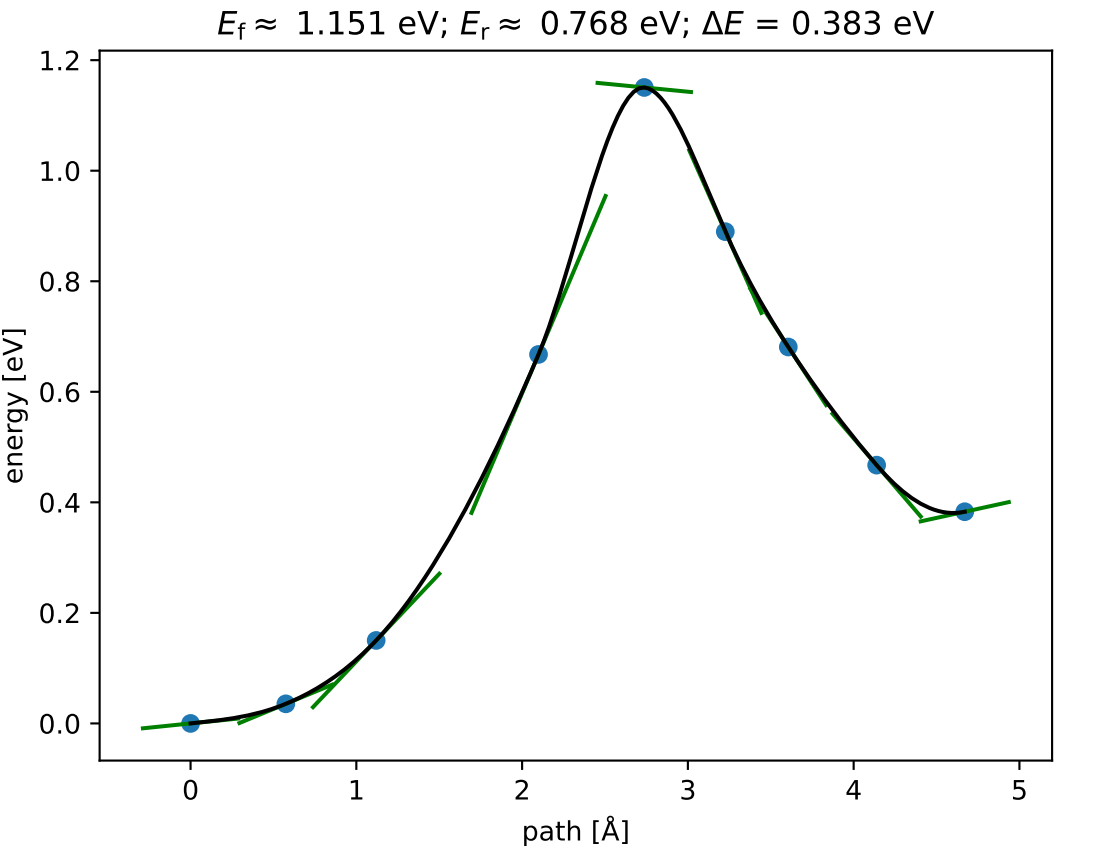
2
3
4
5


$E_f \approx$ 1.151 eV; $E_r \approx$ 0.768 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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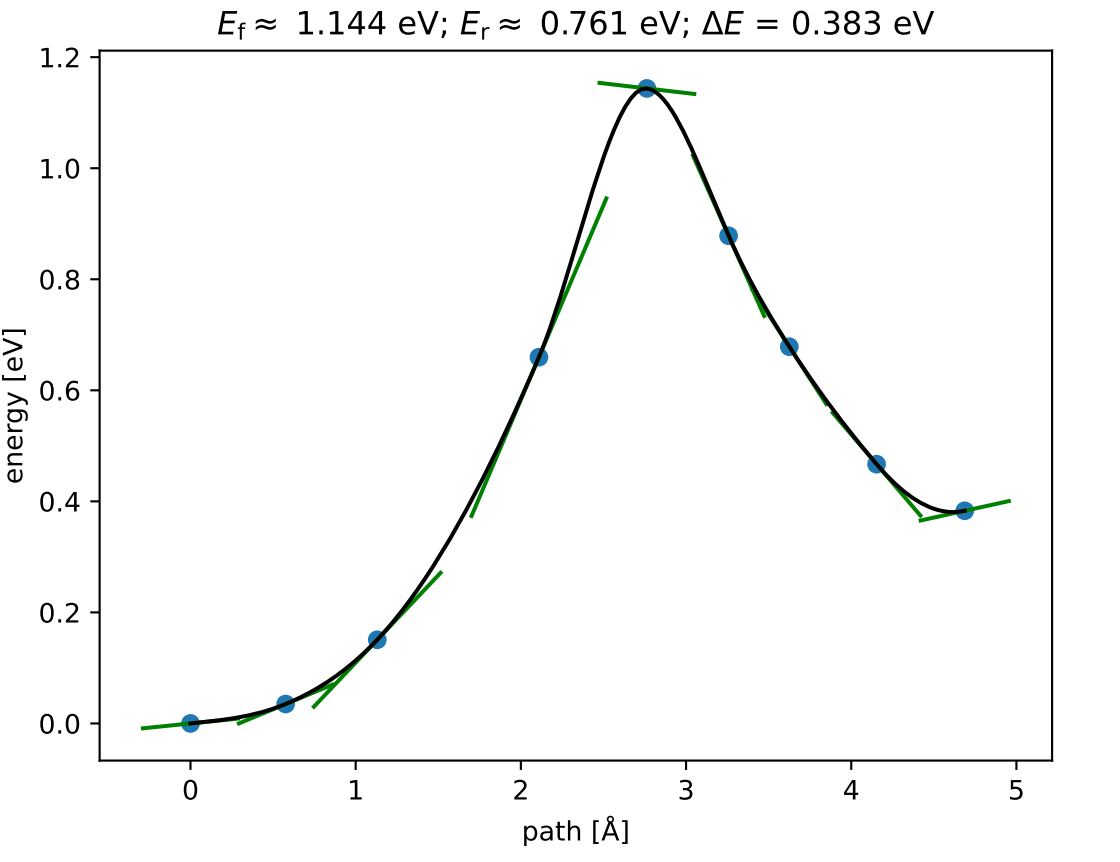
2
3
4
5


$E_f \approx$ 1.144 eV; $E_r \approx$ 0.761 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.8
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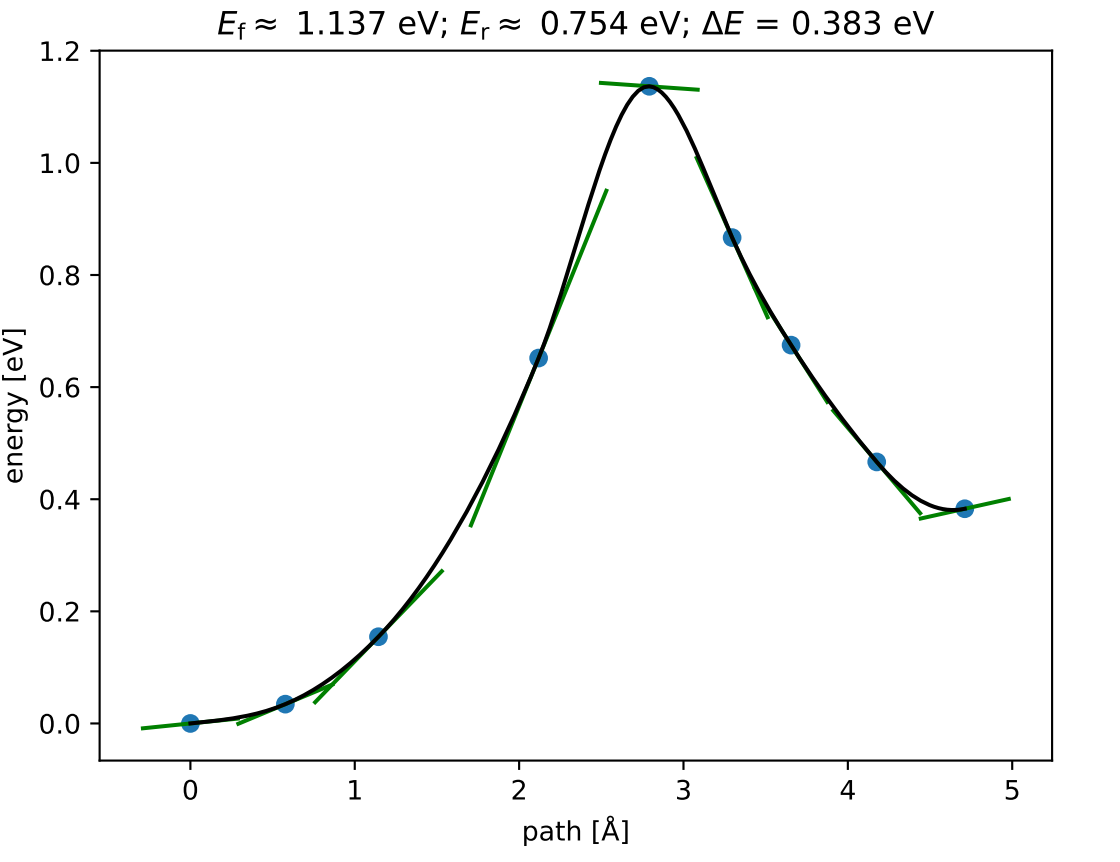
2
3
4
5


$E_f \approx$ 1.137 eV; $E_r \approx$ 0.754 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.4
0.6
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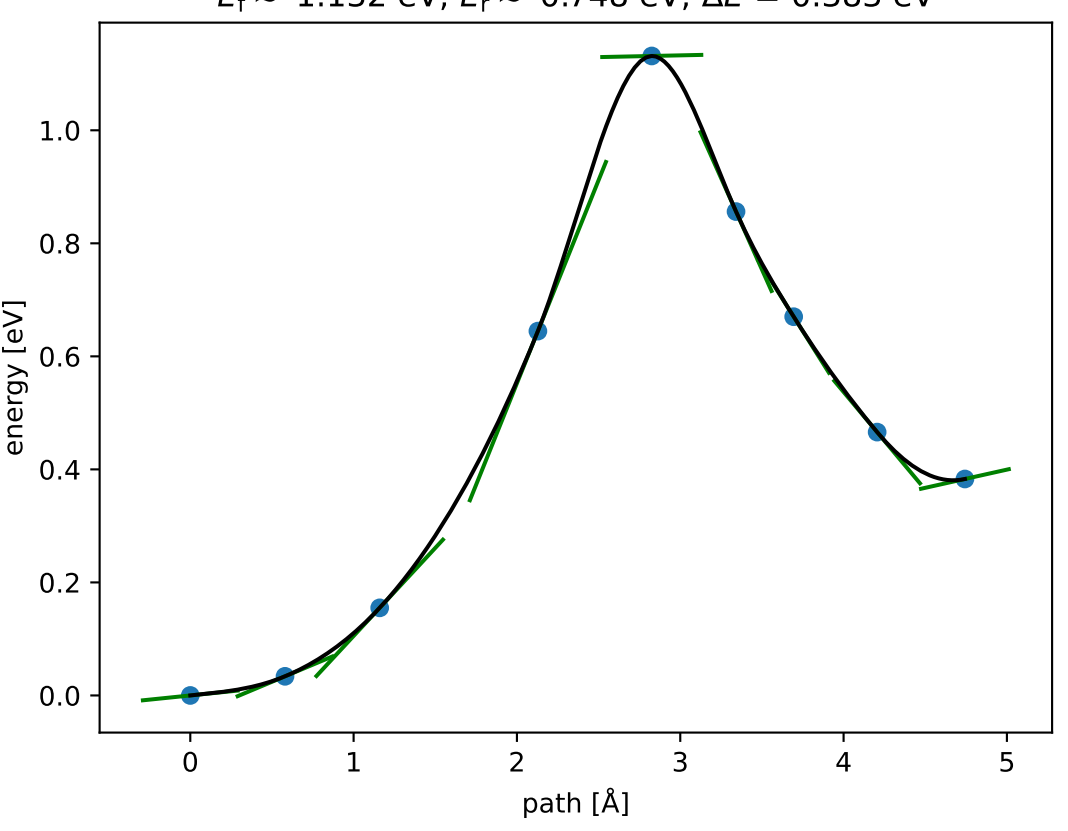
2
3
4
5


$E_f \approx$ 1.132 eV; $E_r \approx$ 0.748 eV; ΔE = 0.383 eV
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path [Å]
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0.8
1.0
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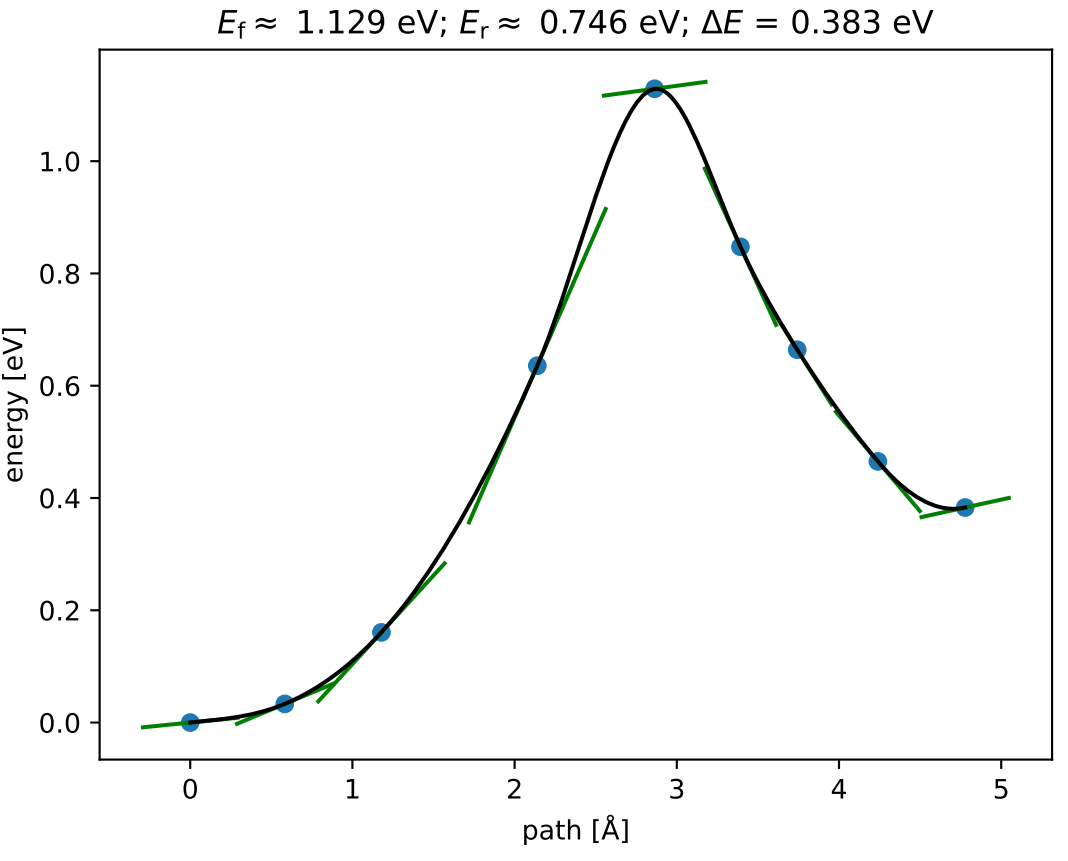
2
3
4
5


$E_f \approx$ 1.129 eV; $E_r \approx$ 0.746 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.6
0.8
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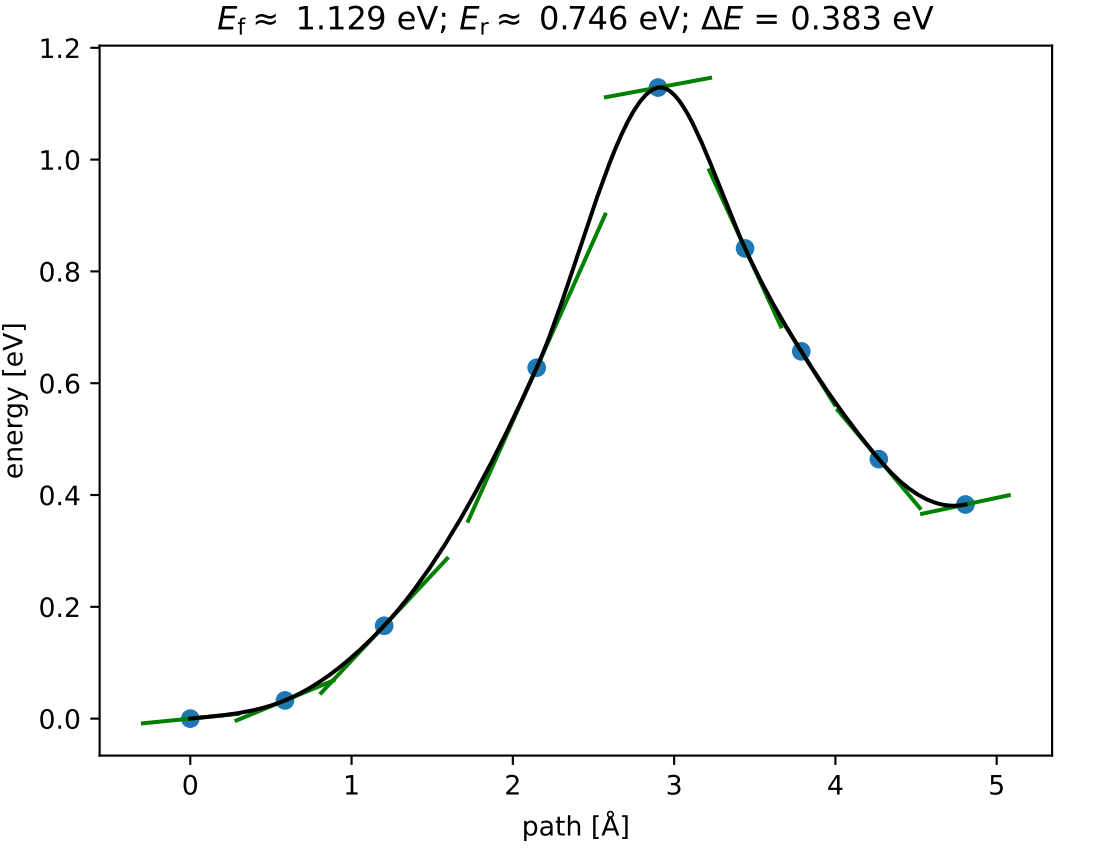
0
1
2
3
4
5


$E_f \approx$ 1.129 eV; $E_r \approx$ 0.746 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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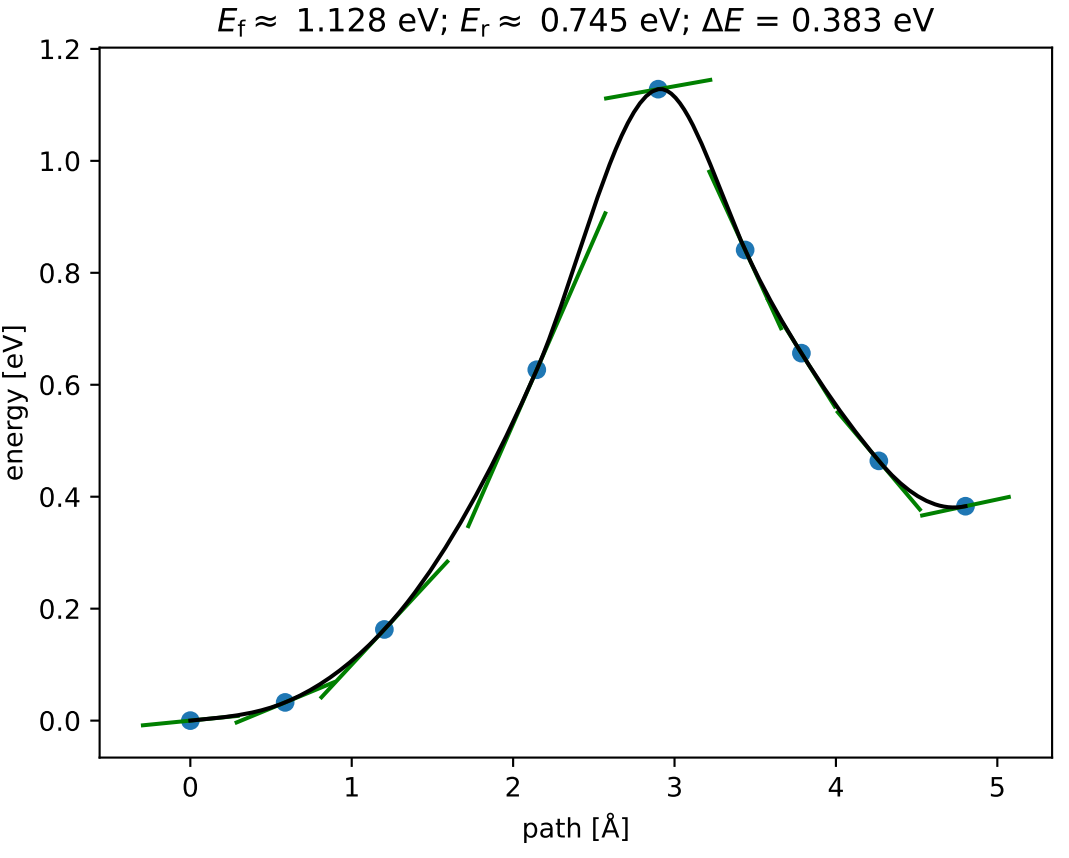
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.128 eV; $E_r \approx$ 0.745 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.4
0.6
0.8
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1.2
0
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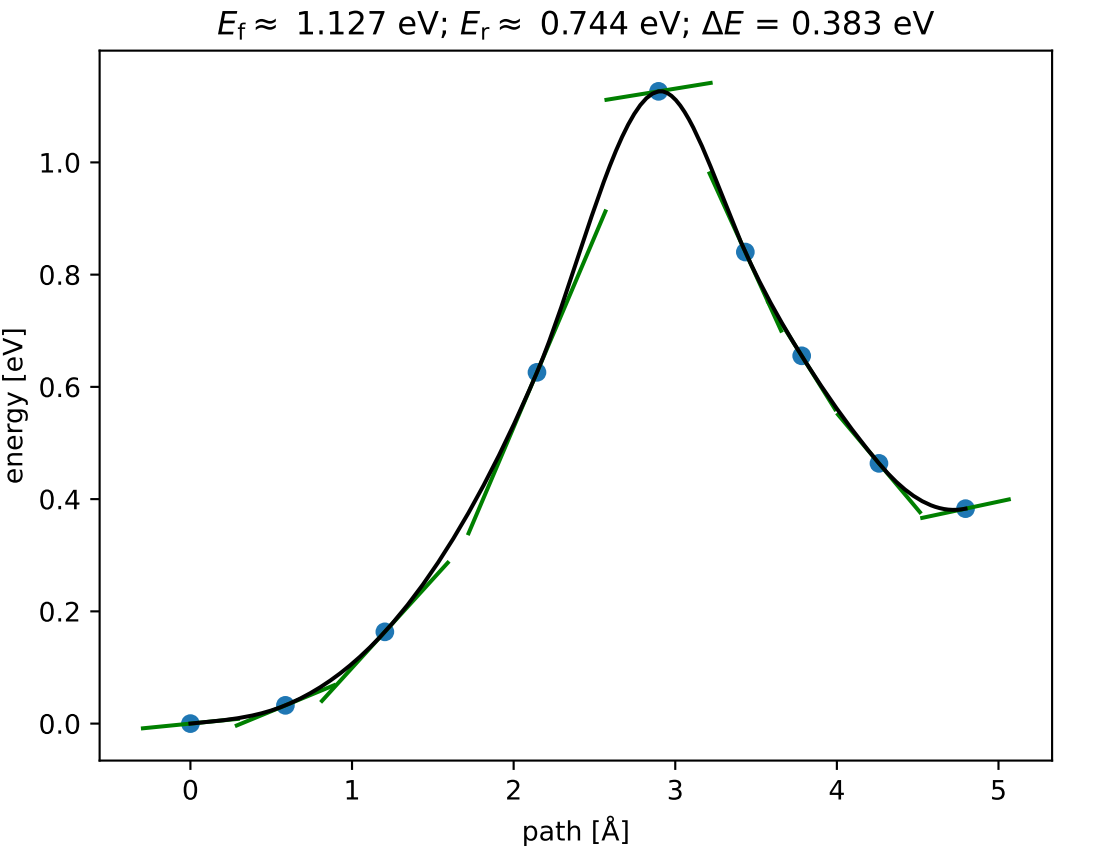
2
3
4
5


$E_f \approx$ 1.127 eV; $E_r \approx$ 0.744 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.4
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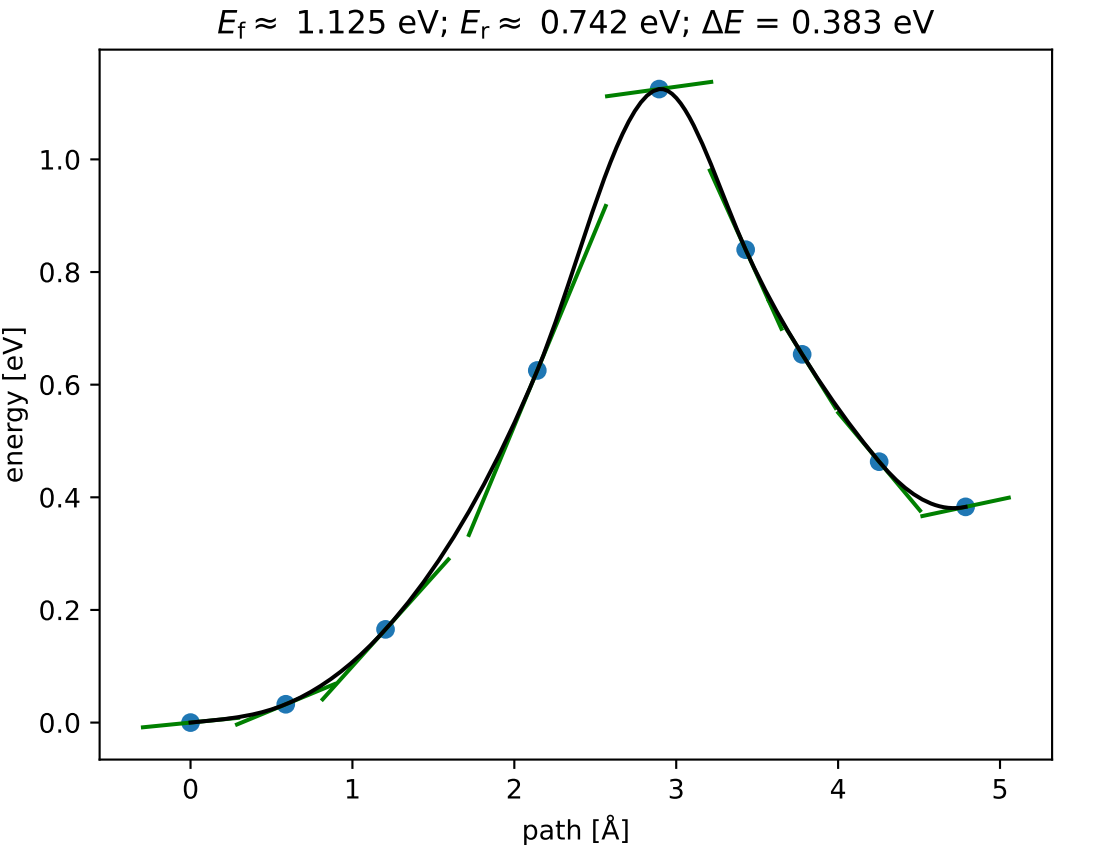
0.8
1.0
0
1
2
3
4
5


$E_f \approx$ 1.125 eV; $E_r \approx$ 0.742 eV; ΔE = 0.383 eV
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path [Å]
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0.8
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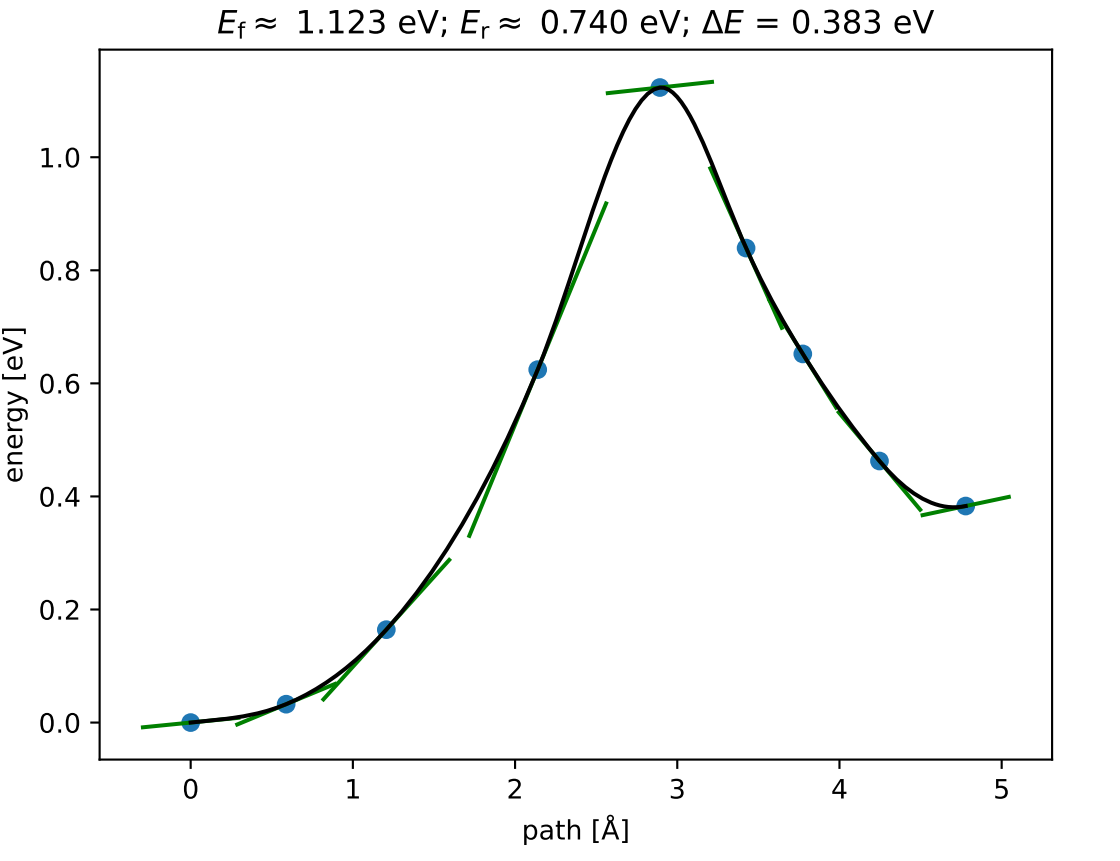
2
3
4
5


$E_f \approx$ 1.123 eV; $E_r \approx$ 0.740 eV; ΔE = 0.383 eV
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path [Å]
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2
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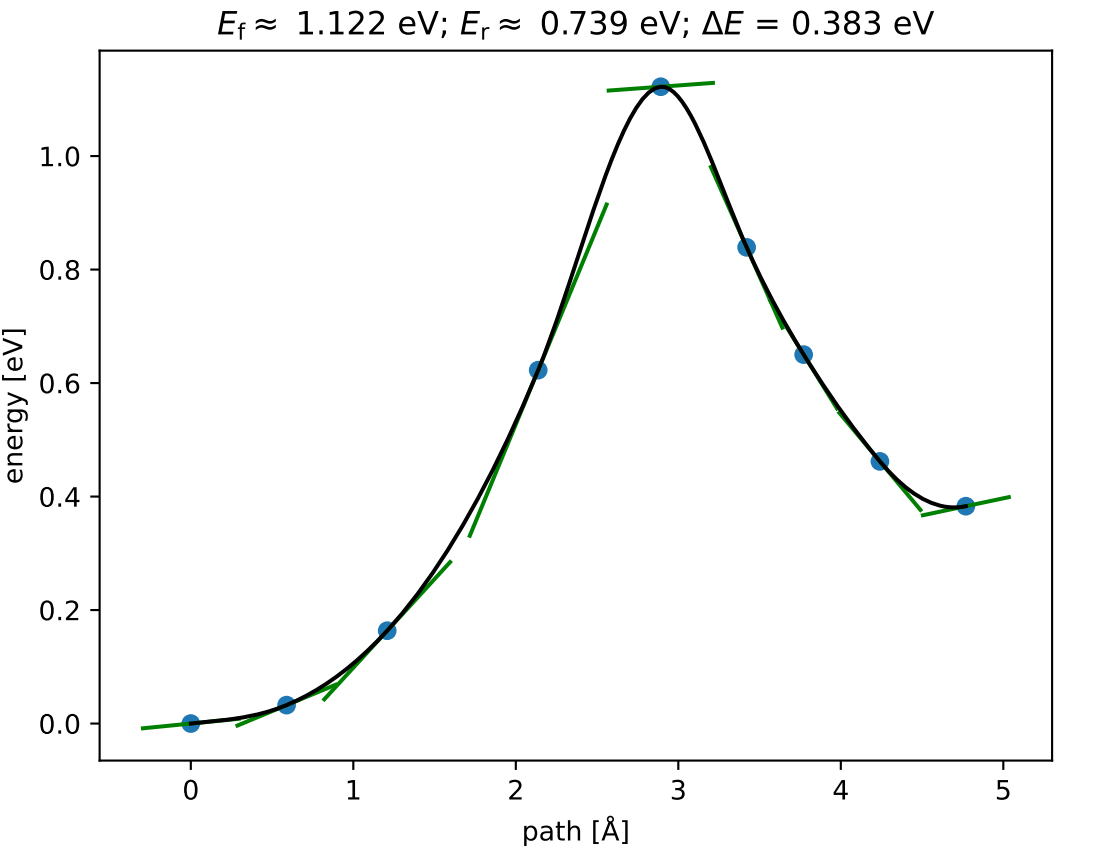
4
5


$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
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2
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4
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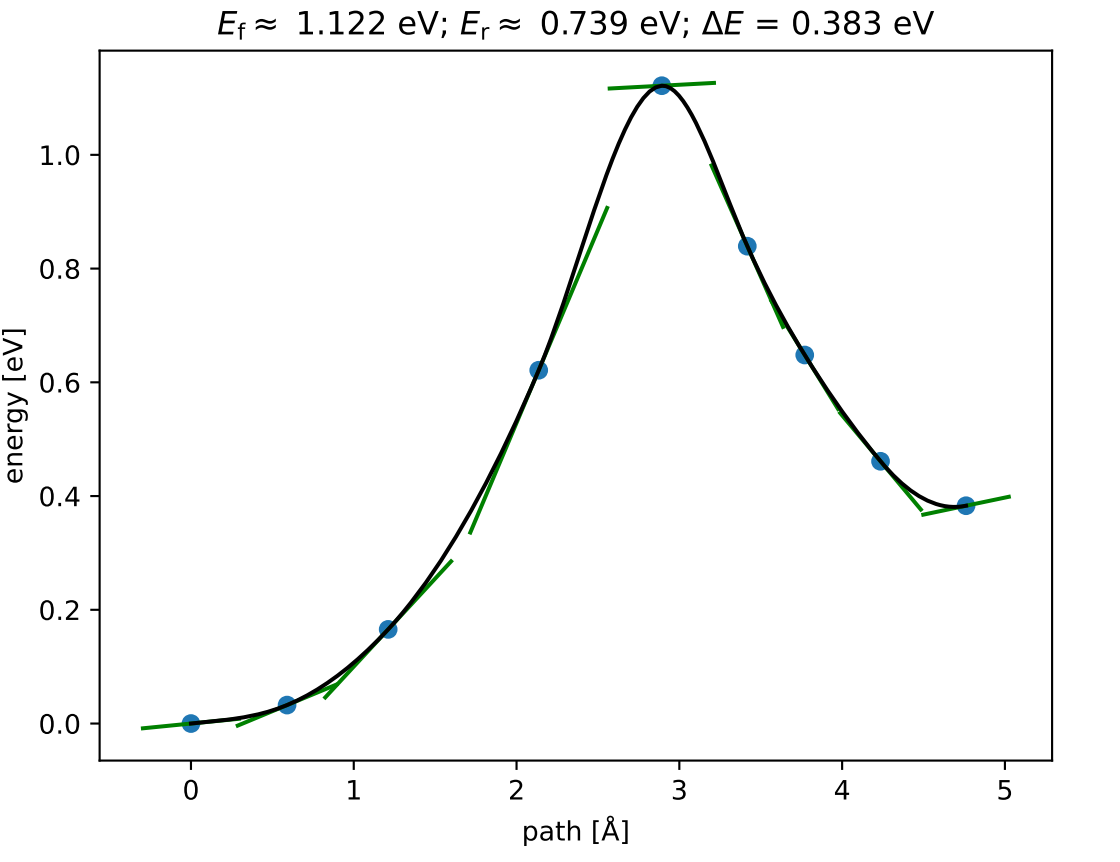
$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
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path [Å]
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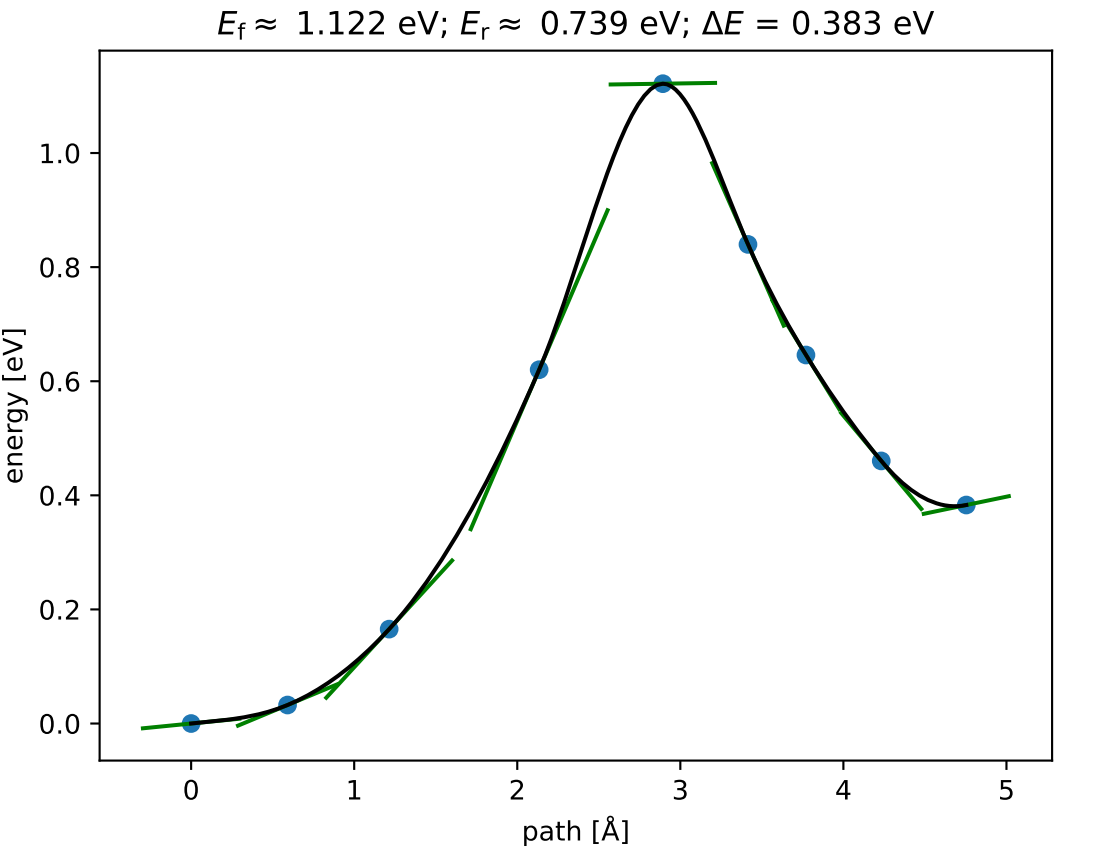
2
3
4
5


$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.8
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2
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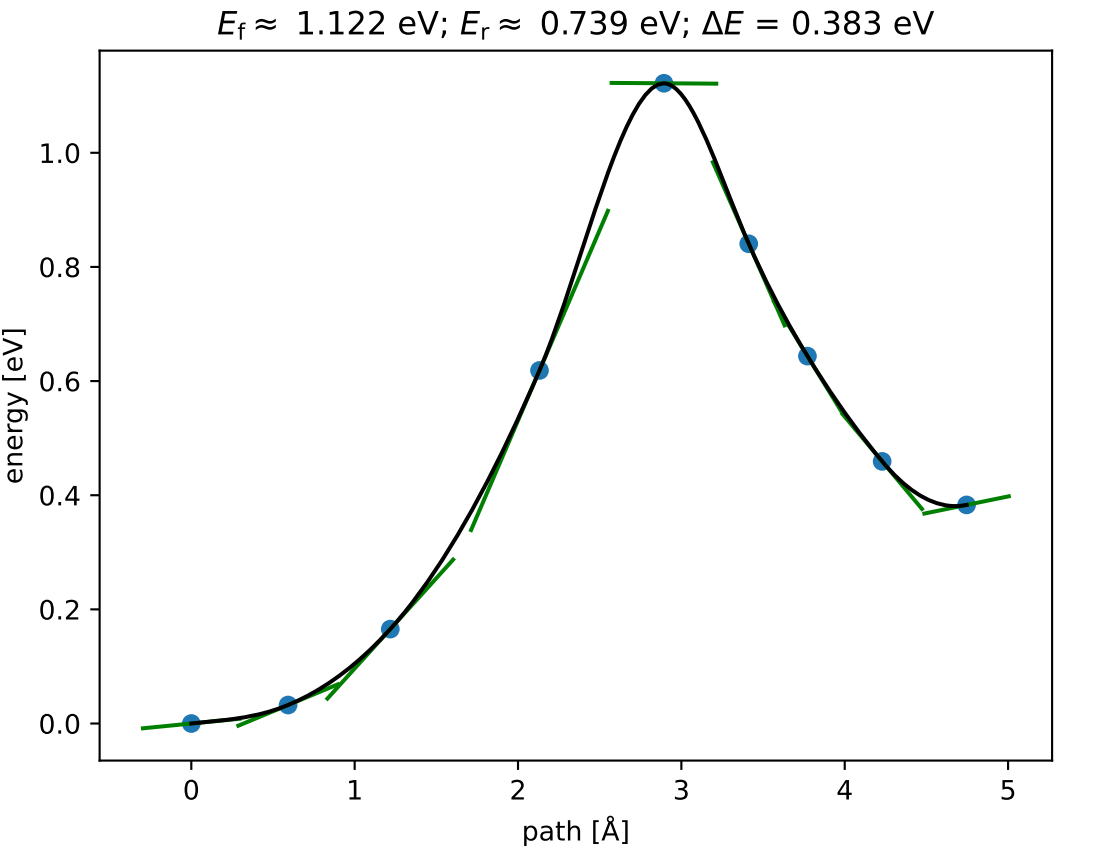
4
5


$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.4
0.6
0.8
1.0
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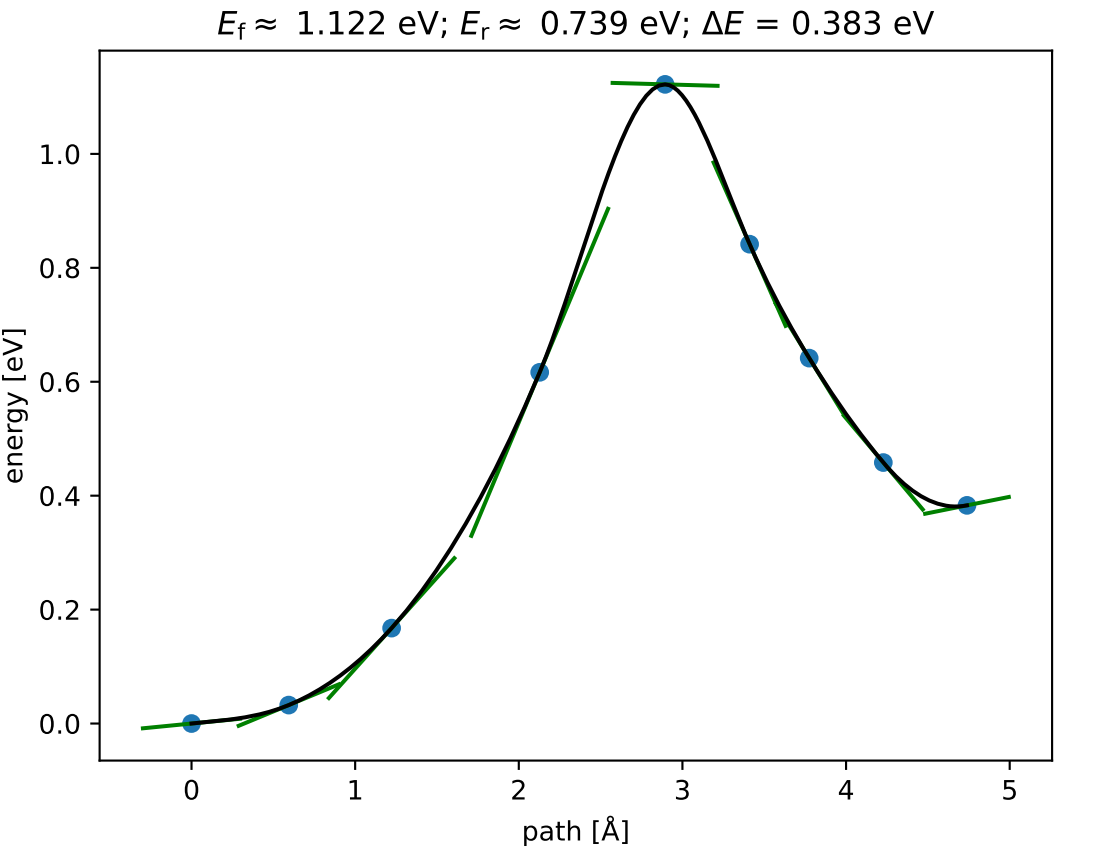
2
3
4
5


$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.4
0.6
0.8
1.0
0
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2
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4
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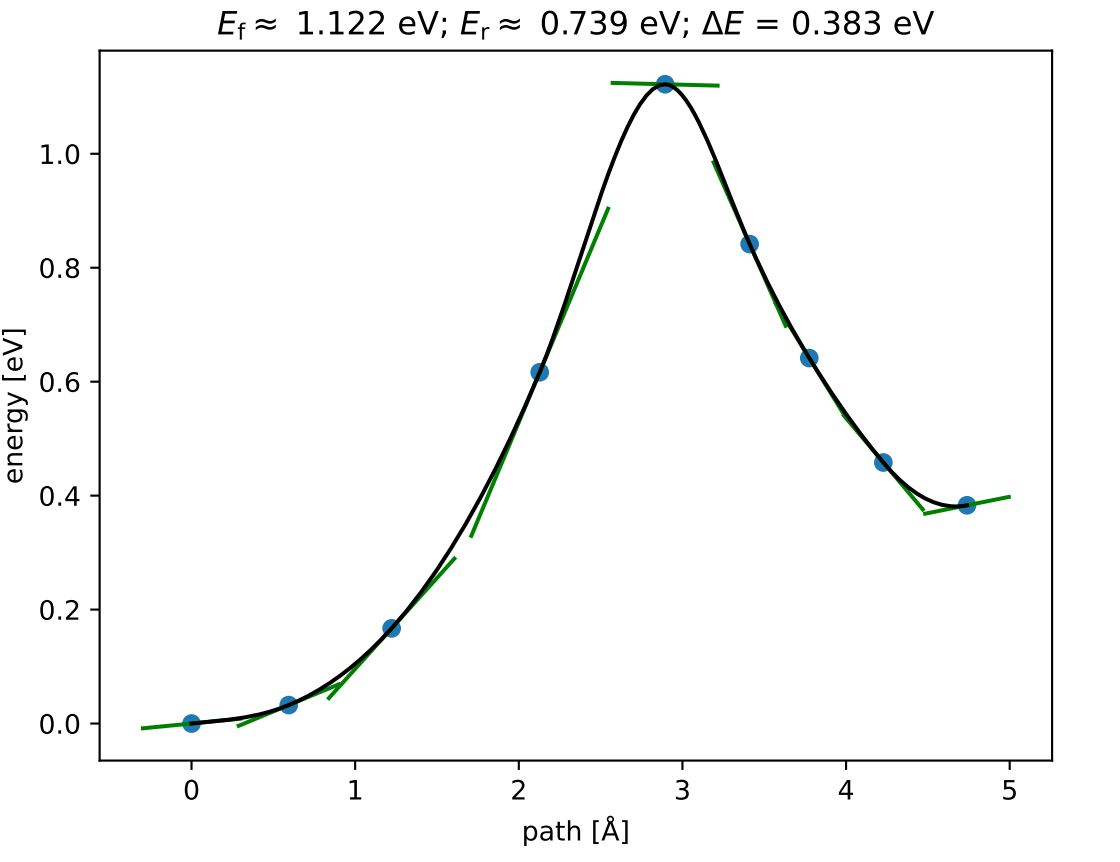
$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.2
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0.8
1.0
0
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2
3
4
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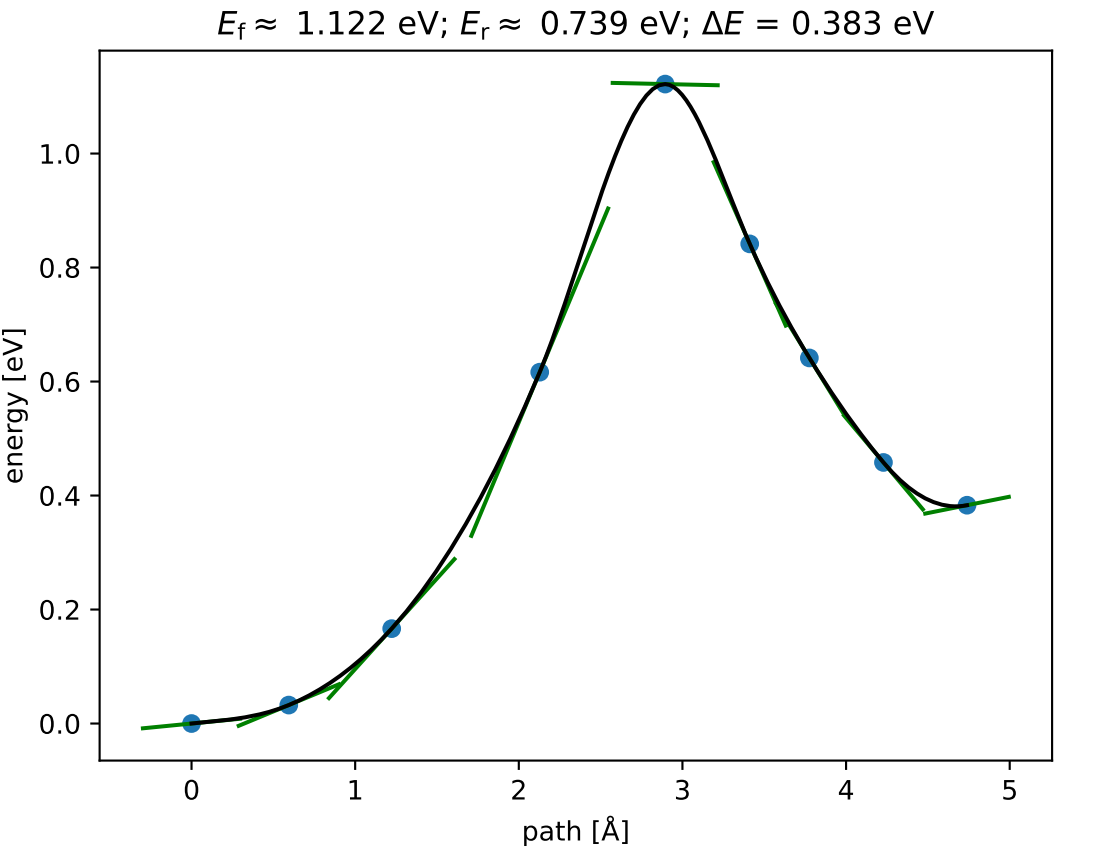
$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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2
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4
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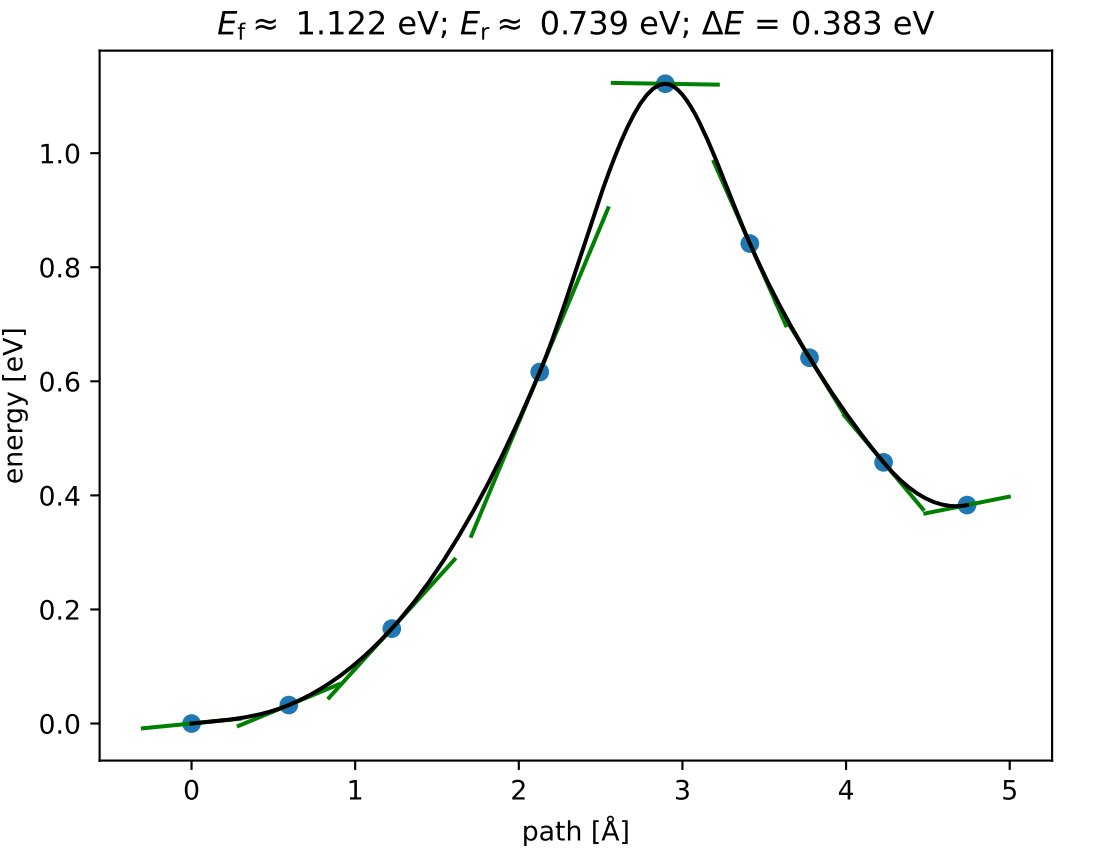
$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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2
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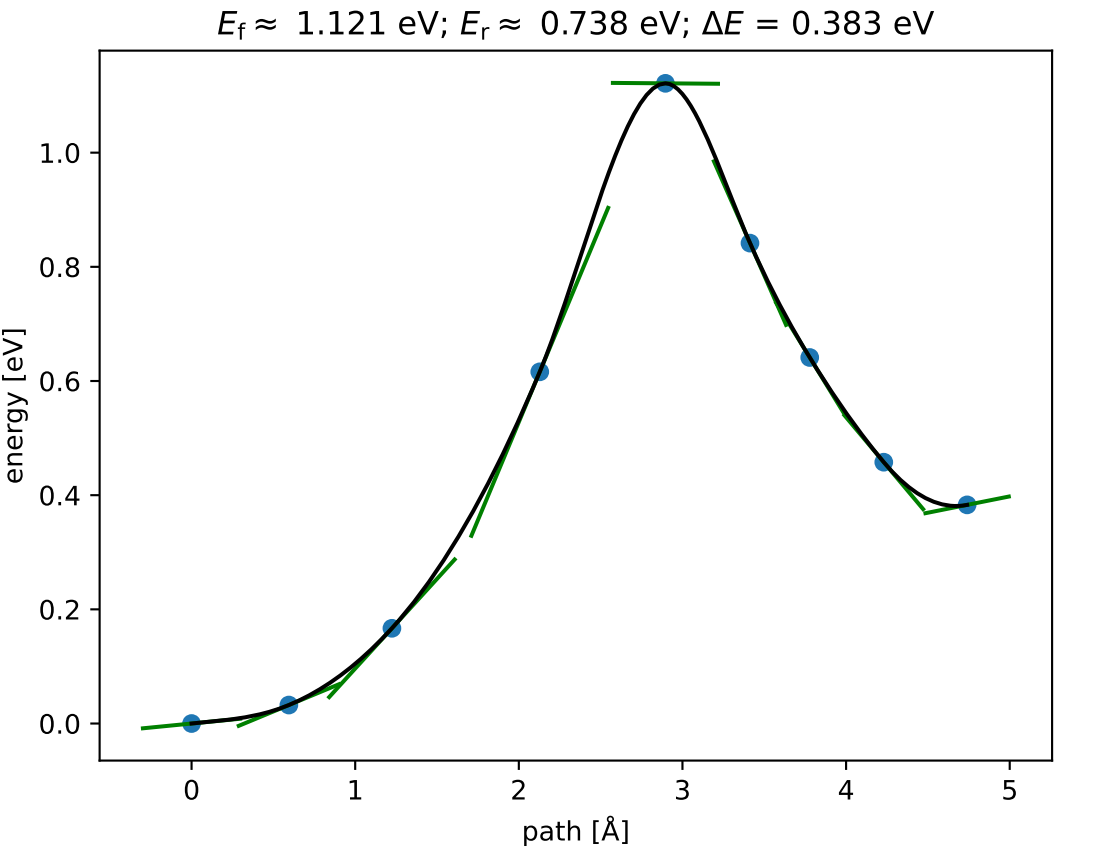
$E_f \approx$ 1.121 eV; $E_r \approx$ 0.738 eV; ΔE = 0.383 eV
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path [Å]
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2
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4
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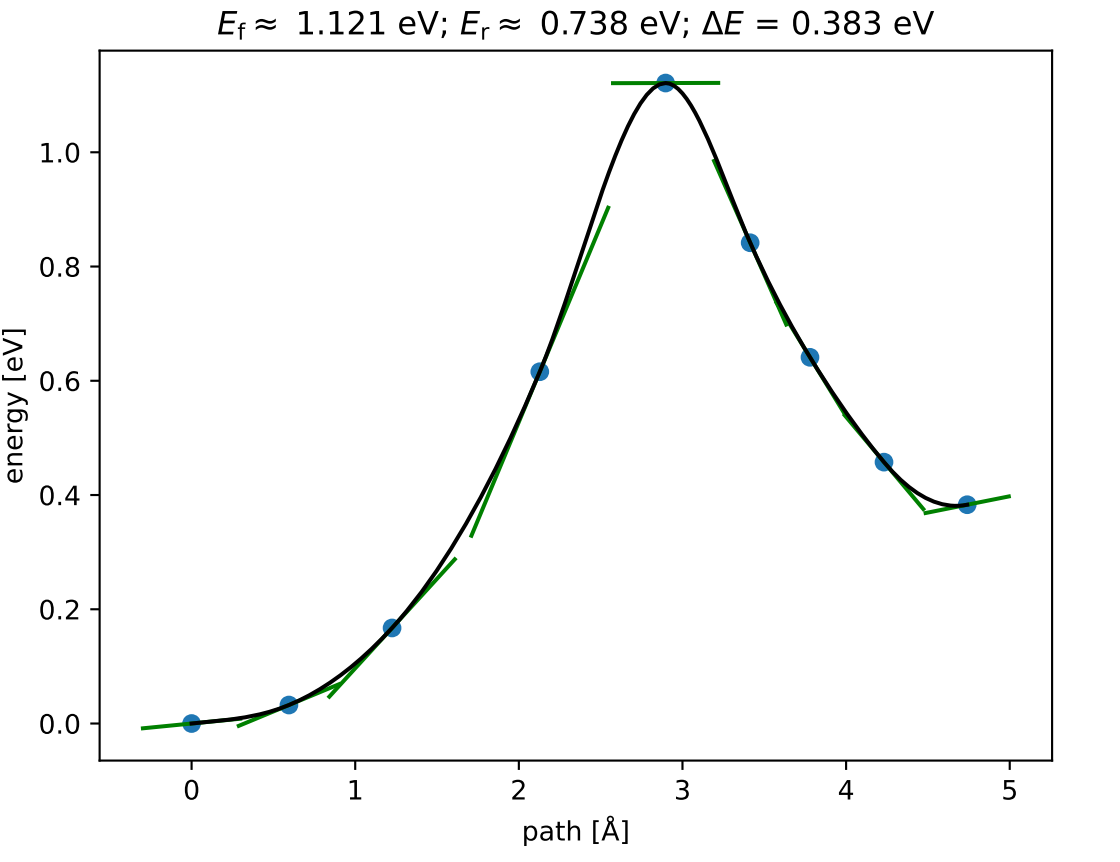
$E_f \approx$ 1.121 eV; $E_r \approx$ 0.738 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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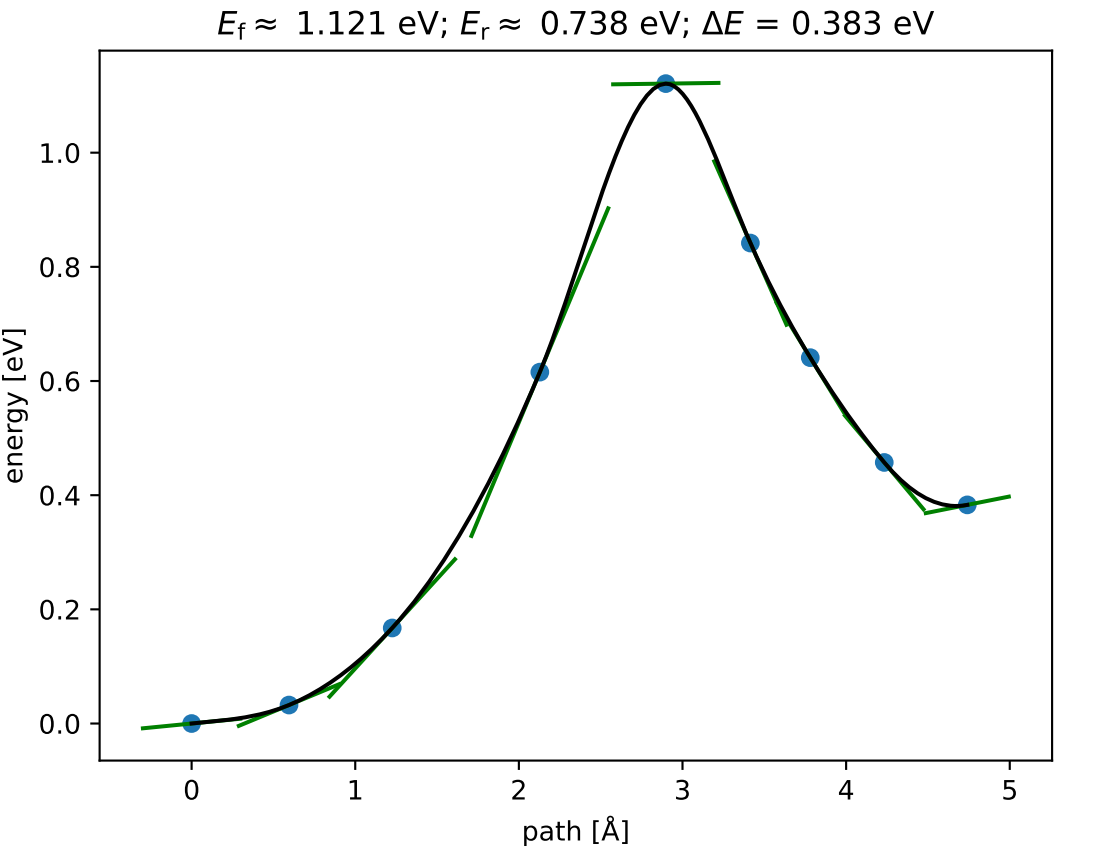
0.2
0.4
0.6
0.8
1.0
0
1
2
3
4
5


$E_f \approx$ 1.121 eV; $E_r \approx$ 0.738 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.2
0.4
0.6
0.8
1.0
0
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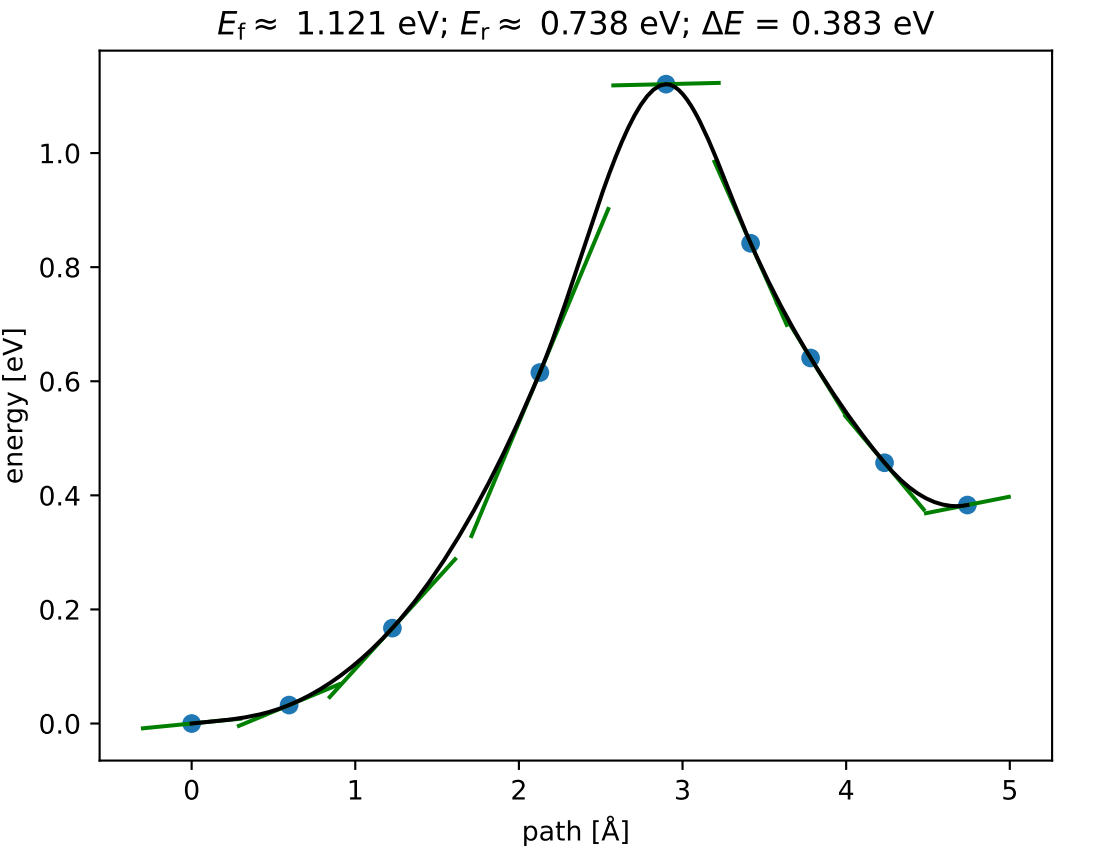
2
3
4
5


$E_f \approx$ 1.121 eV; $E_r \approx$ 0.738 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.4
0.6
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2
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4
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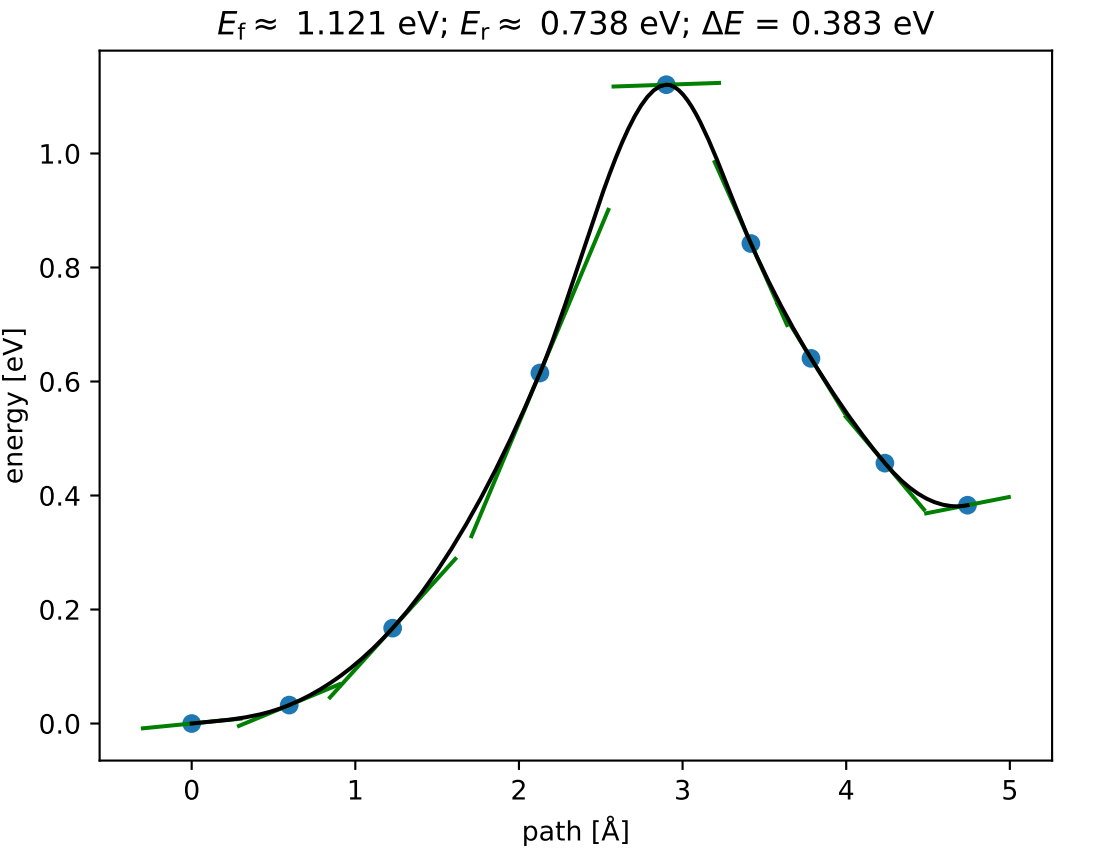
$E_f \approx$ 1.121 eV; $E_r \approx$ 0.738 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.2
0.4
0.6
0.8
1.0
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2
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5