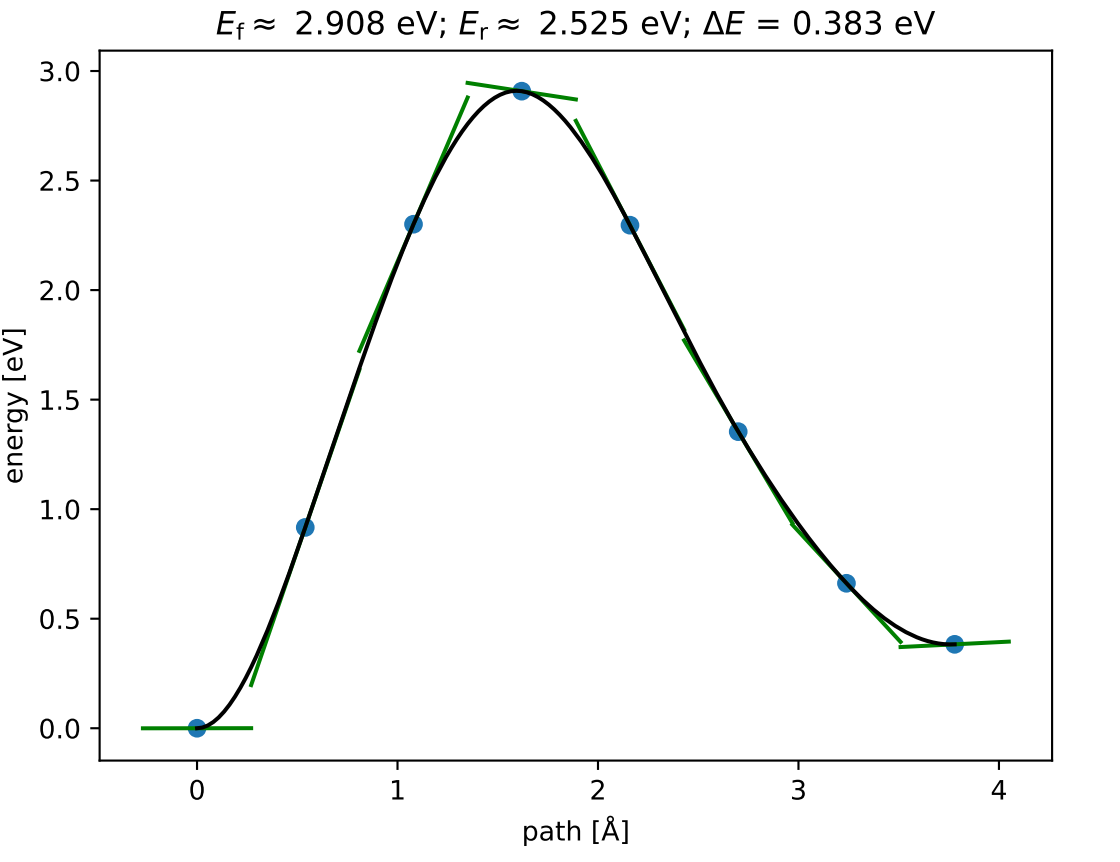
$E_f \approx$ 2.908 eV; $E_r \approx$ 2.525 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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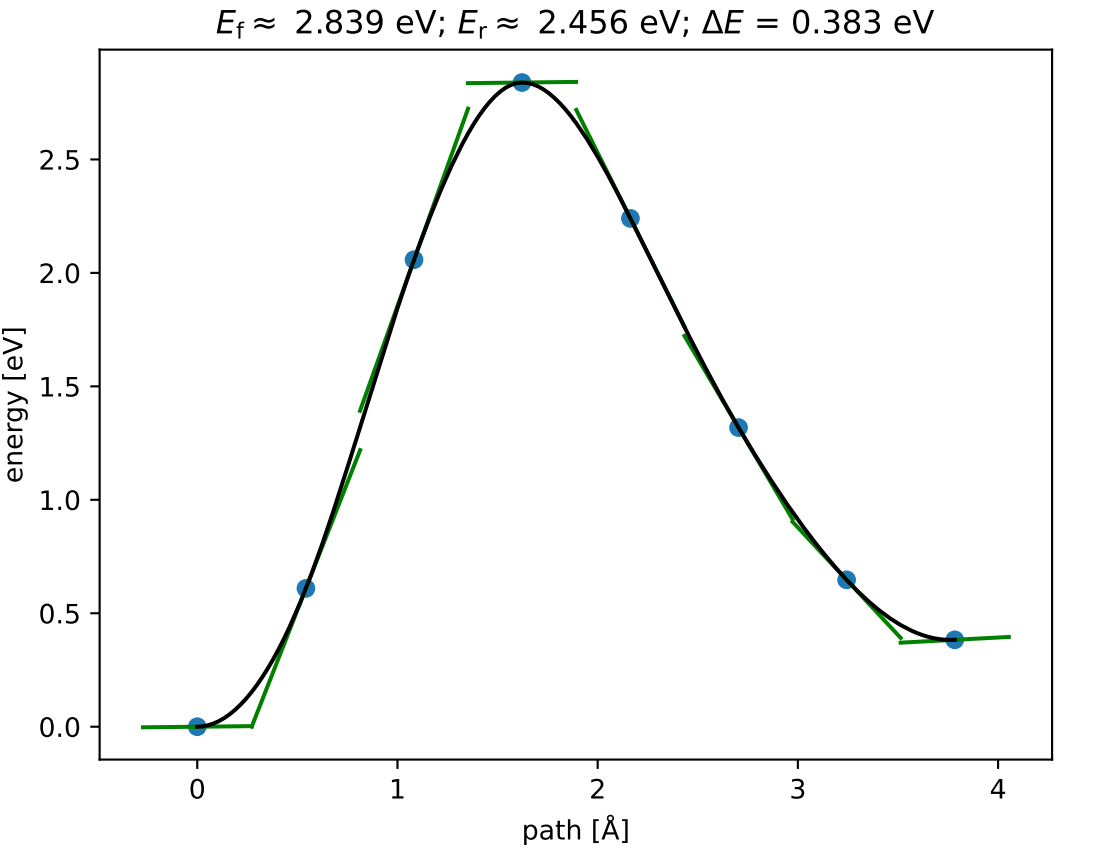
0.5
1.0
1.5
2.0
2.5
3.0
0
1
2
3
4


$E_f \approx$ 2.839 eV; $E_r \approx$ 2.456 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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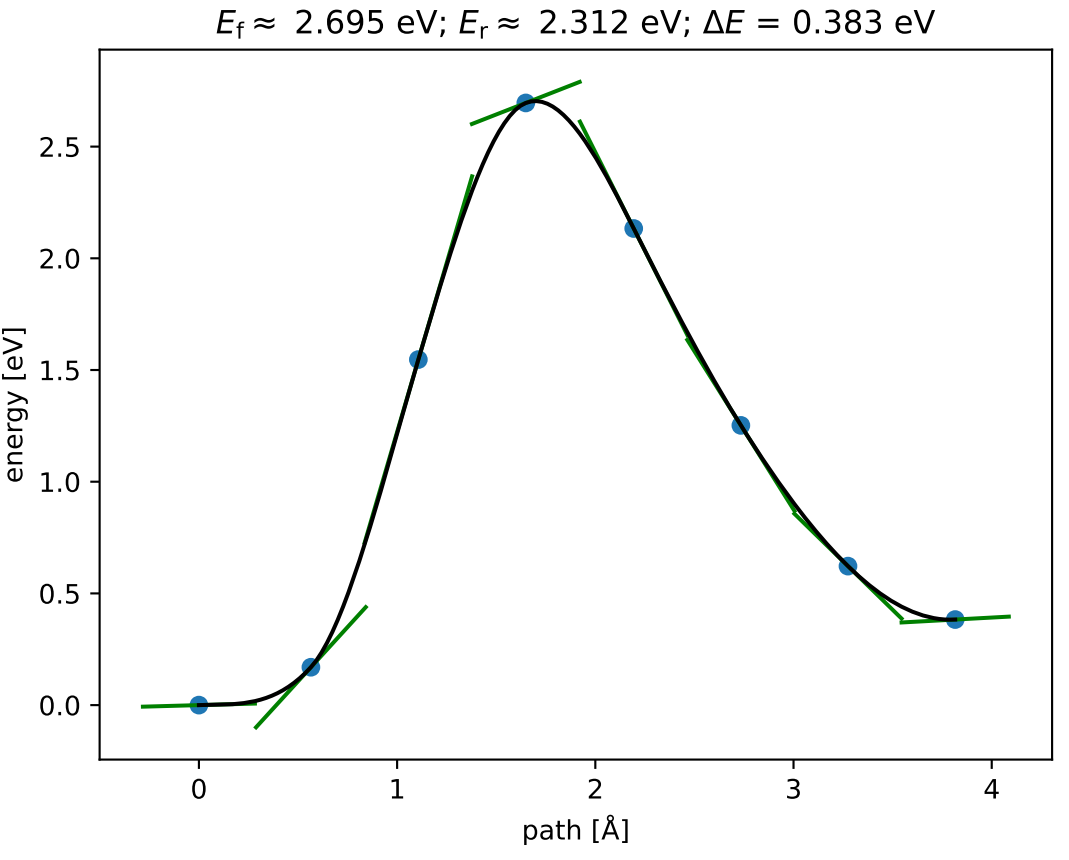
0.5
1.0
1.5
2.0
2.5
0
1
2
3
4


$E_f \approx$ 2.695 eV; $E_r \approx$ 2.312 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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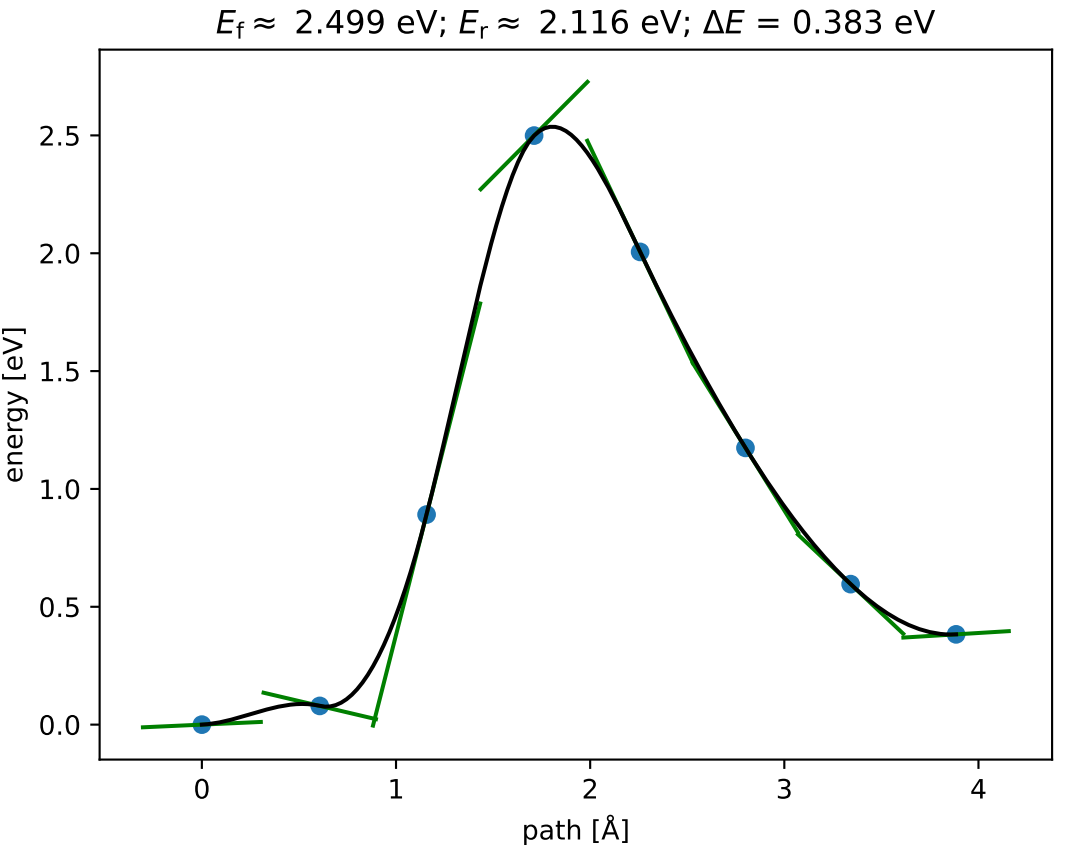
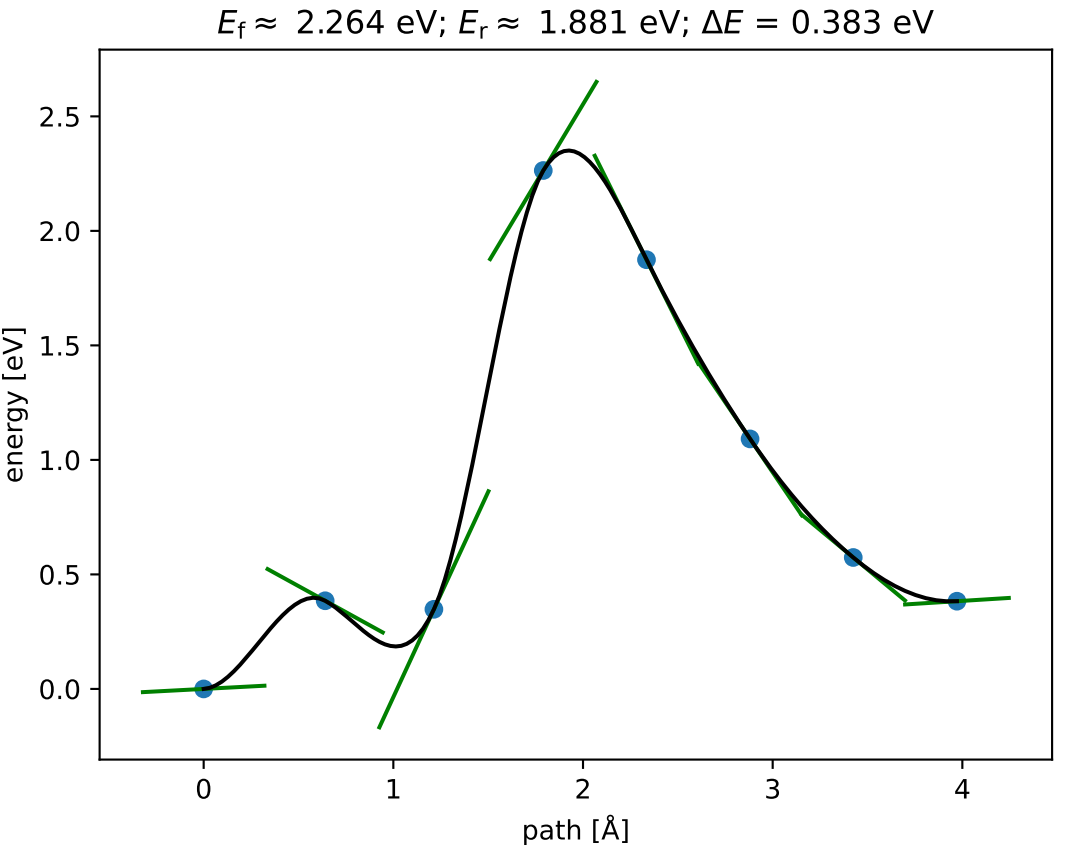
0.5
1.0
1.5
2.0
2.5
0
1
2
3
4


$E_f \approx$ 2.499 eV; $E_r \approx$ 2.116 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


$E_f \approx$ 2.264 eV; $E_r \approx$ 1.881 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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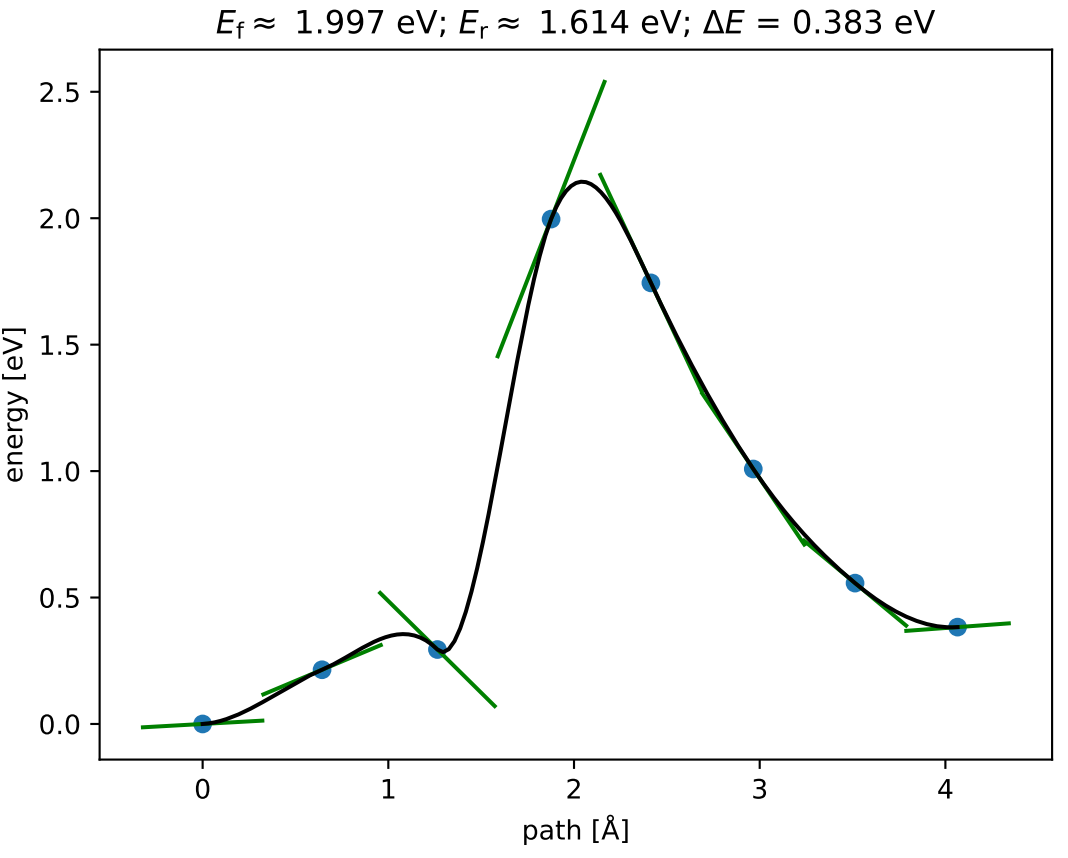
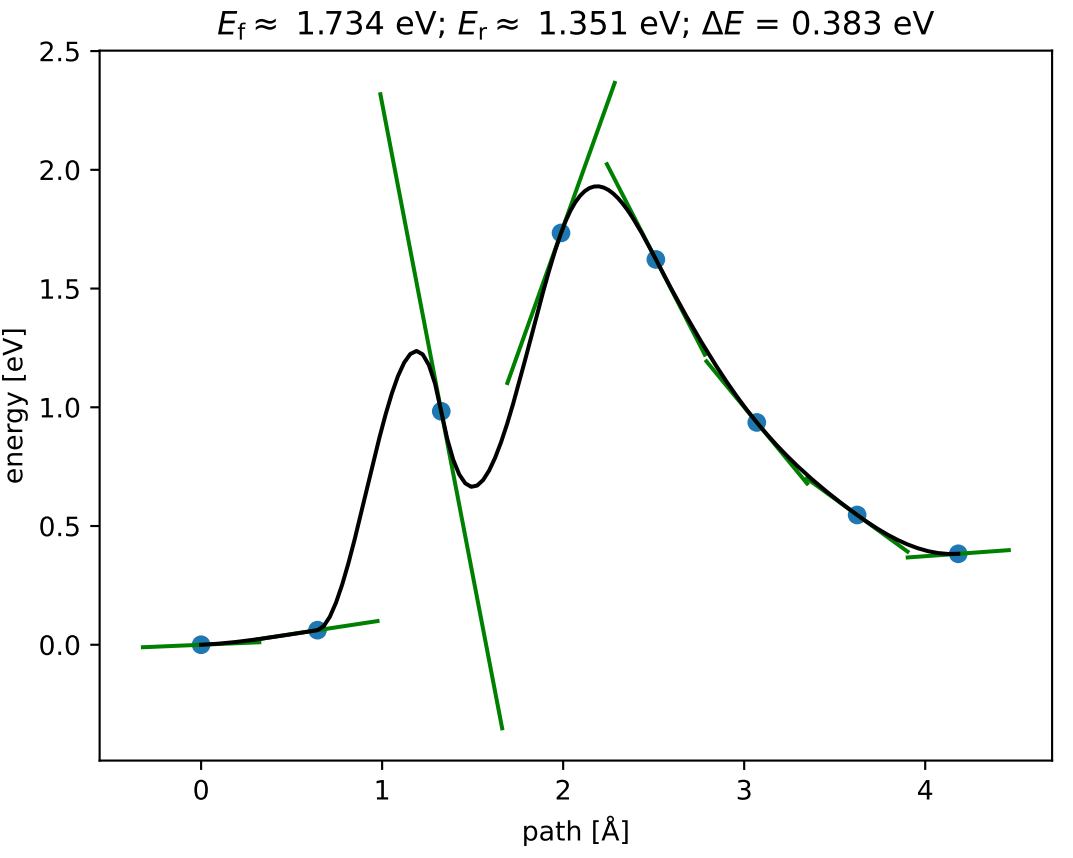
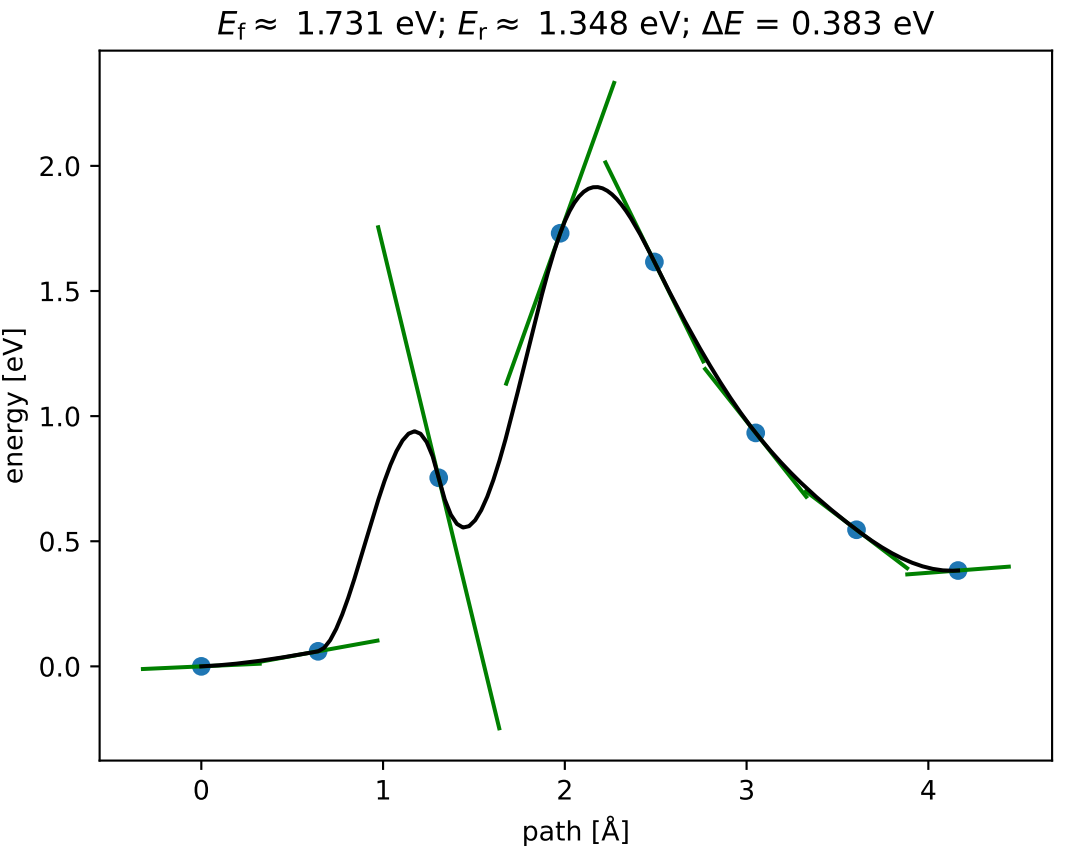
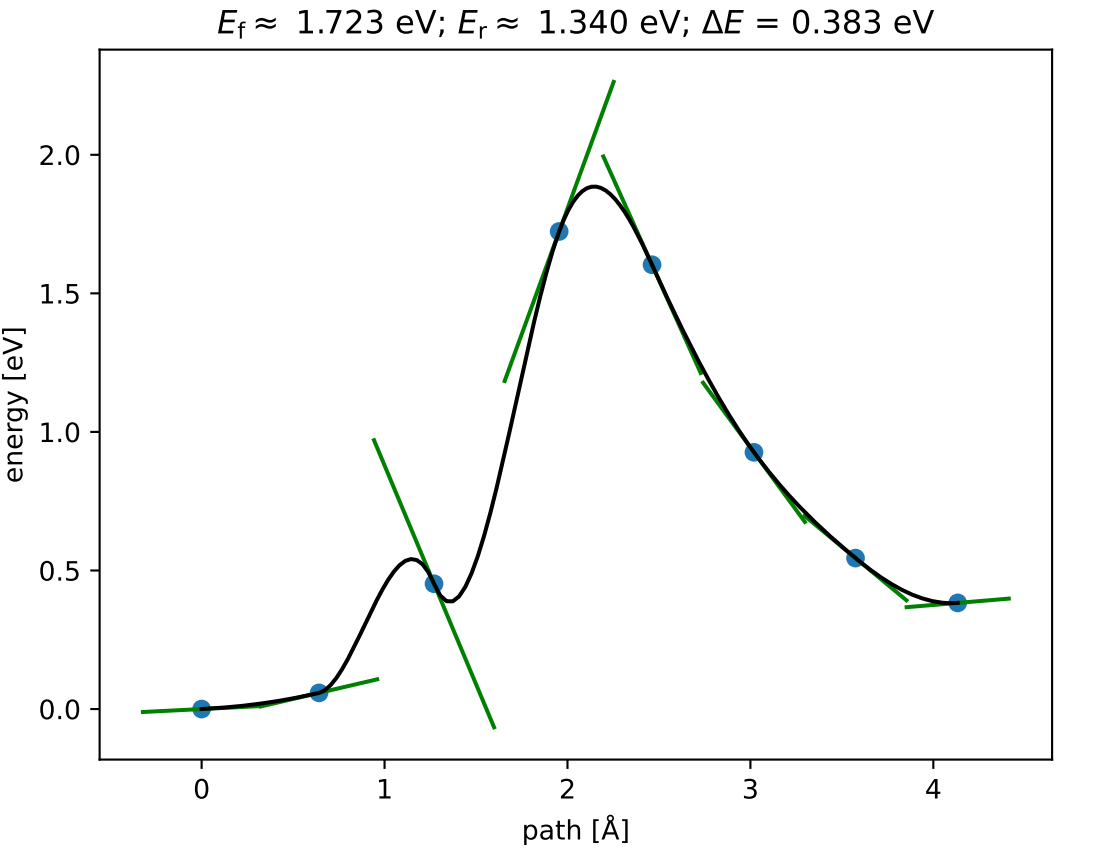
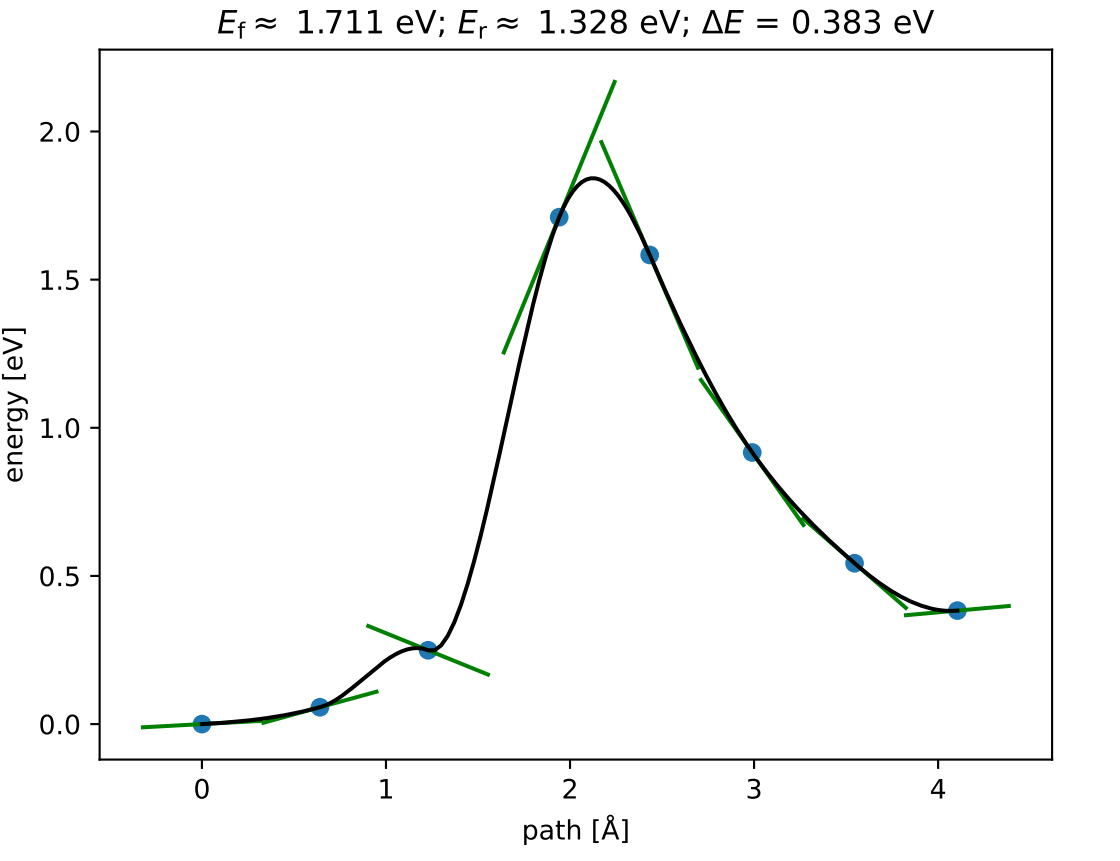
0.5
1.0
1.5
2.0
2.5
0
1
2
3
4

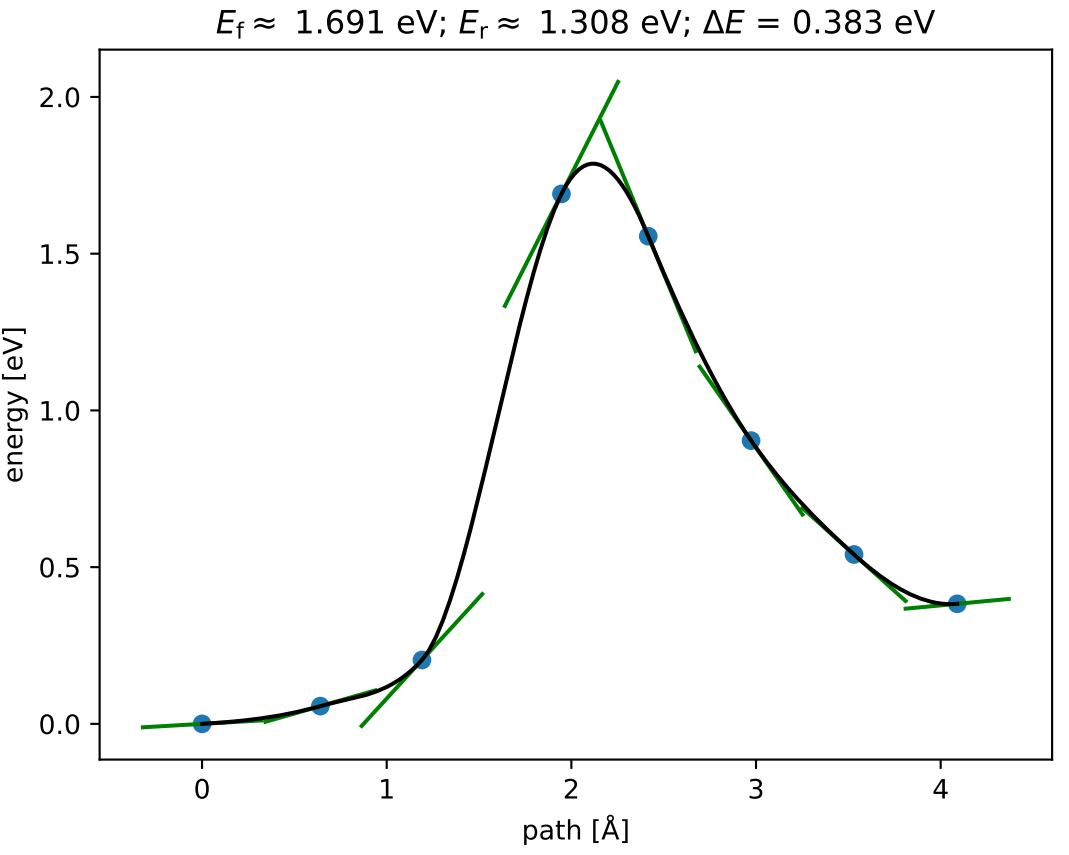

$E_f \approx$ 1.997 eV; $E_r \approx$ 1.614 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
2.5
0
1
2
3
4

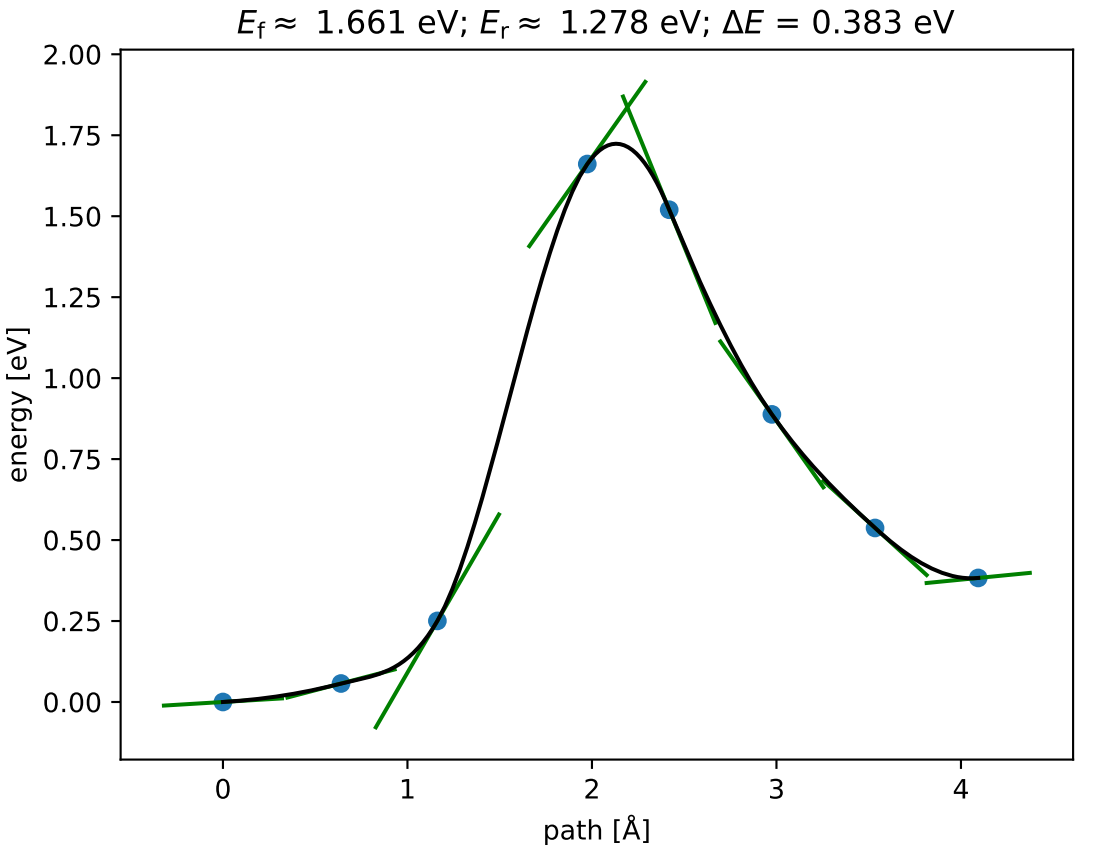

$E_f \approx$ 1.734 eV; $E_r \approx$ 1.351 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
2.5
2.0
1.5
1.0
0.5
0.0
0
1
2
3
4

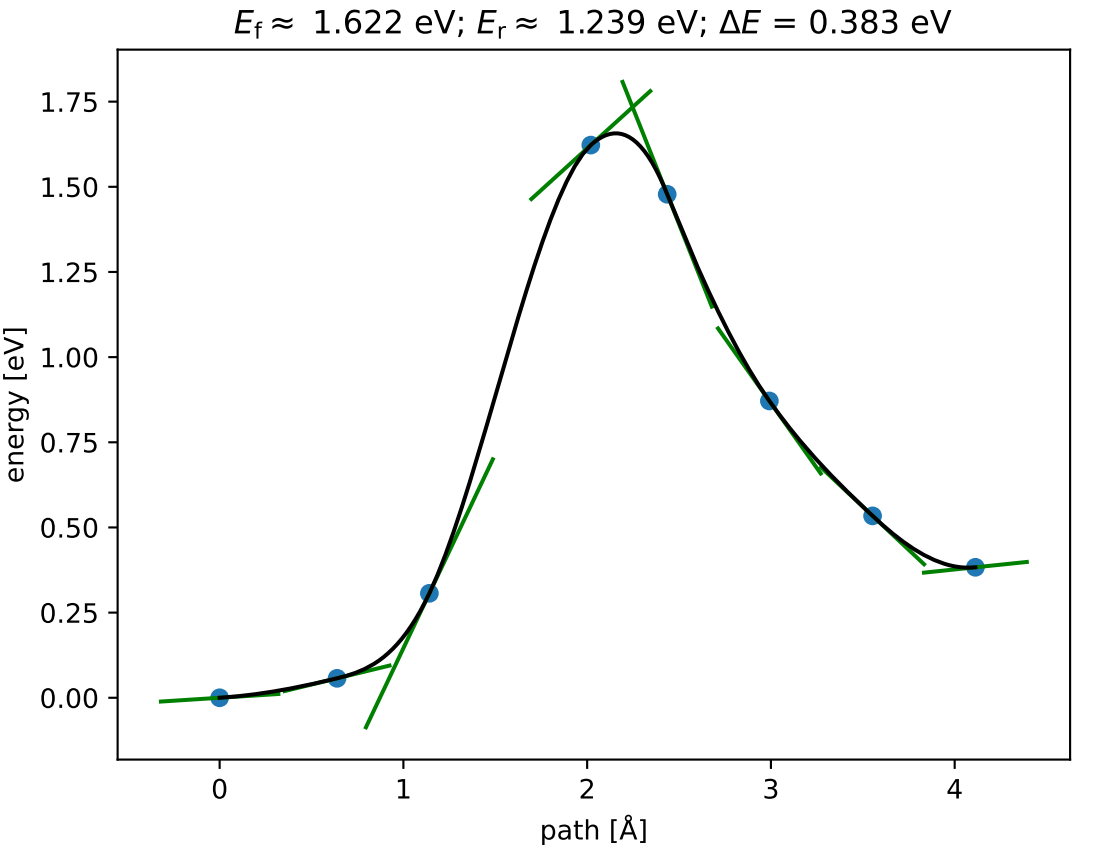

$E_f \approx$ 1.731 eV; $E_r \approx$ 1.348 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4

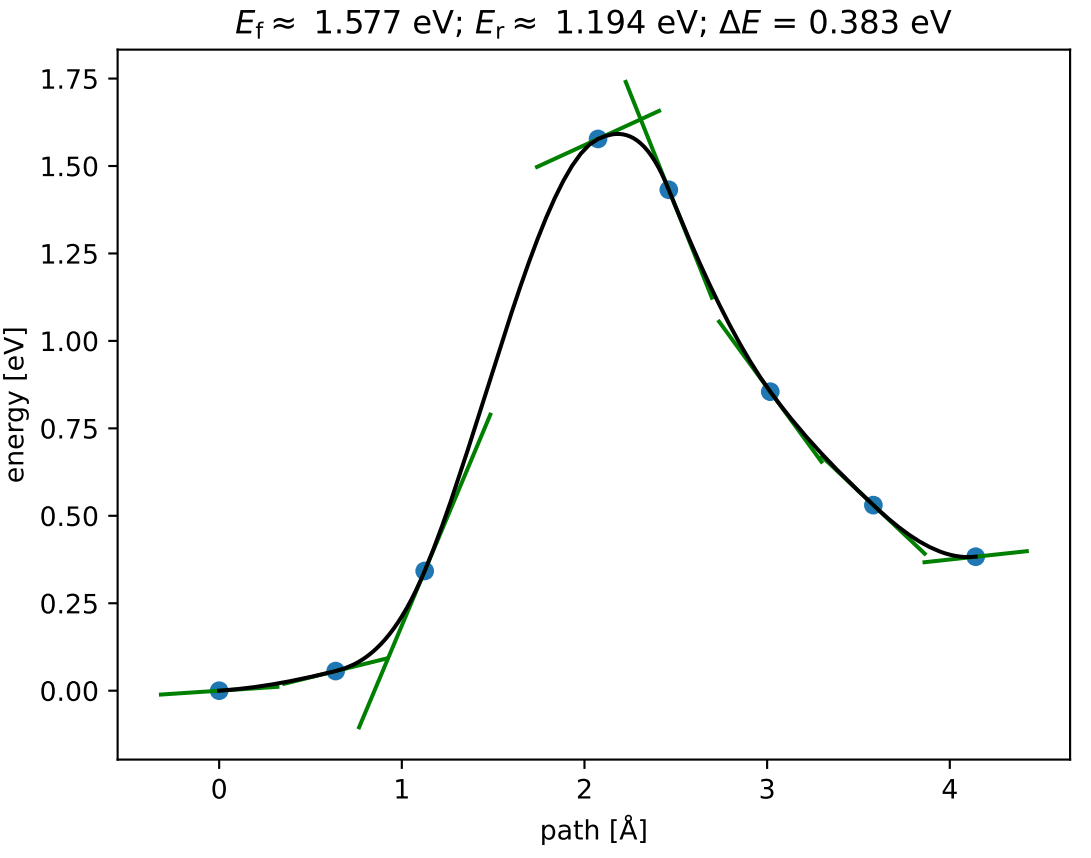

$E_f \approx$ 1.723 eV; $E_r \approx$ 1.340 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4

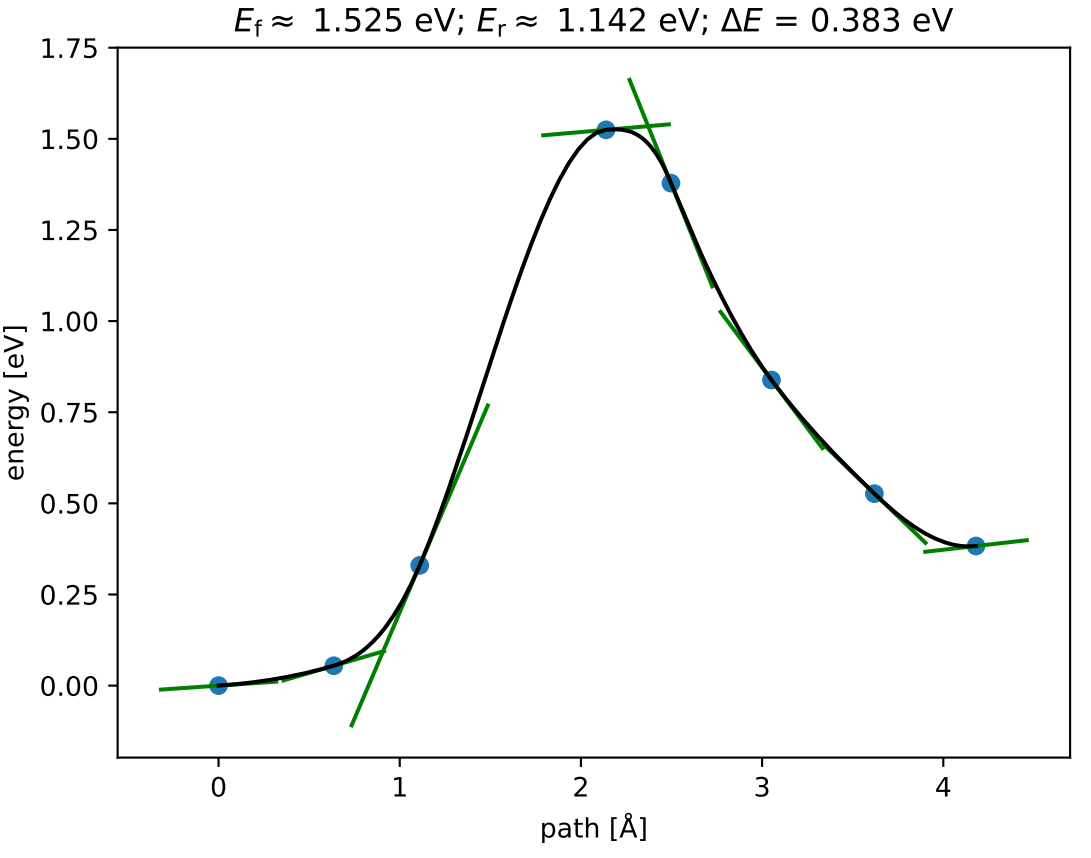

$E_f \approx$ 1.711 eV; $E_r \approx$ 1.328 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4

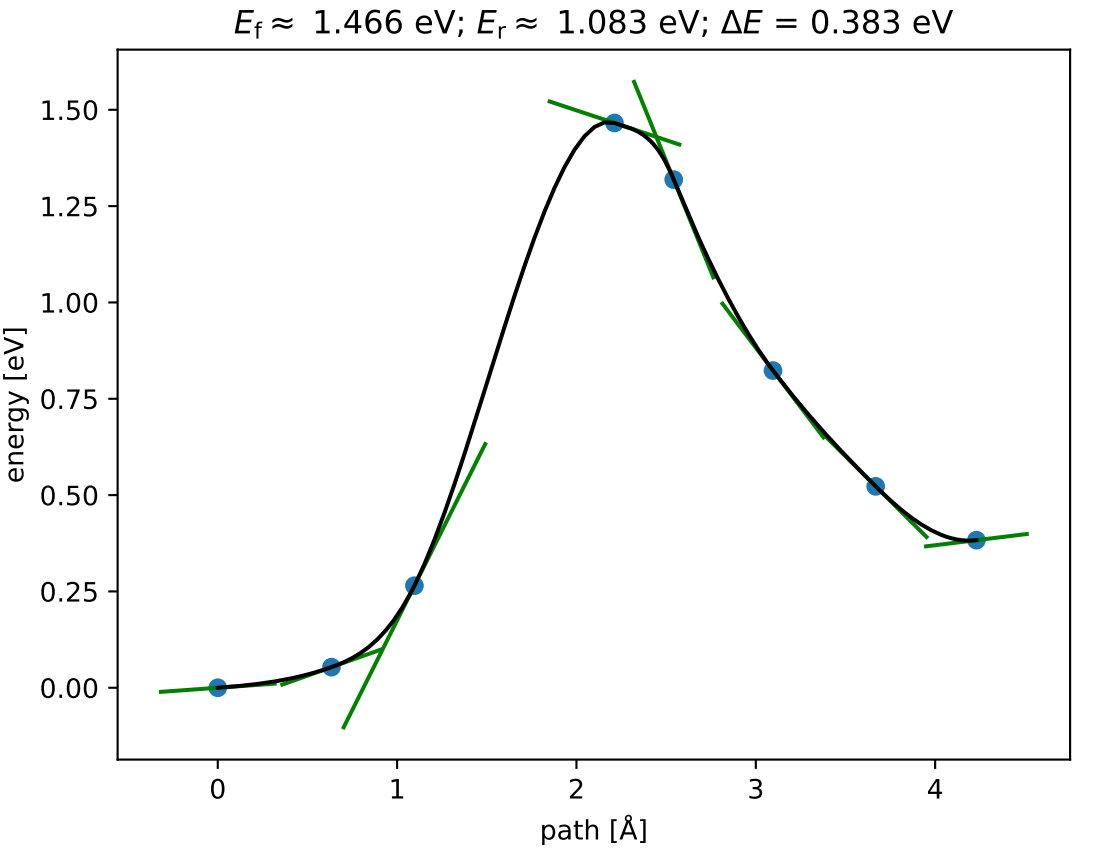

$E_f \approx$ 1.691 eV; $E_r \approx$ 1.308 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4

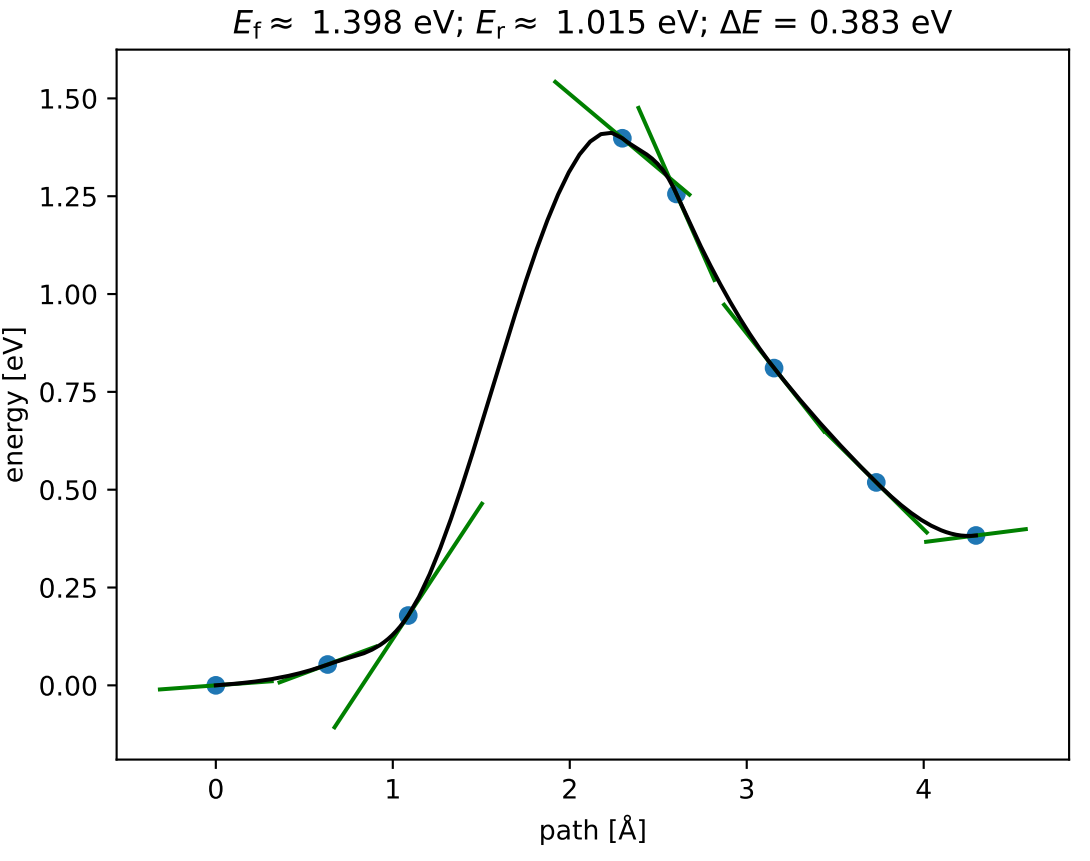

$E_f \approx$ 1.661 eV; $E_r \approx$ 1.278 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4

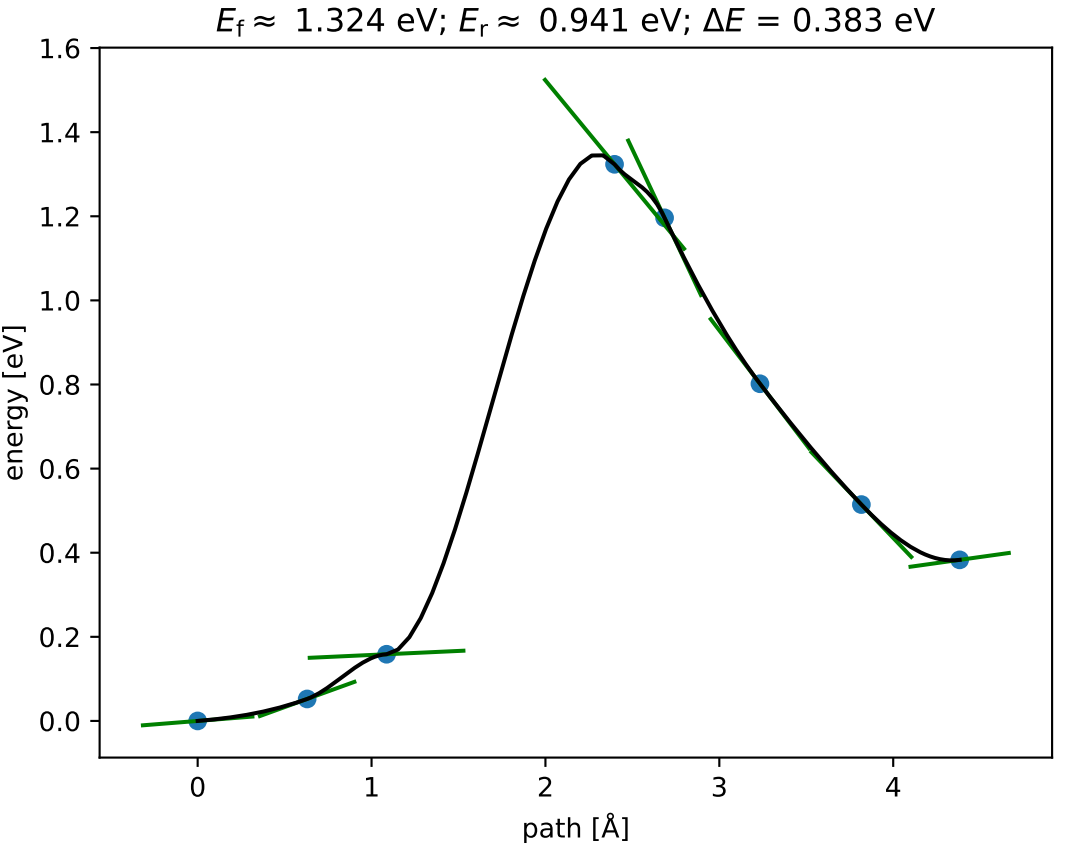

$E_f \approx$ 1.622 eV; $E_r \approx$ 1.239 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
0
1
2
3
4


$E_f \approx$ 1.577 eV; $E_r \approx$ 1.194 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4


$E_f \approx$ 1.525 eV; $E_r \approx$ 1.142 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4


$E_f \approx$ 1.466 eV; $E_r \approx$ 1.083 eV; ΔE = 0.383 eV
energy [eV]
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4
path [Å]


$E_f \approx$ 1.398 eV; $E_r \approx$ 1.015 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4


$E_f \approx$ 1.324 eV; $E_r \approx$ 0.941 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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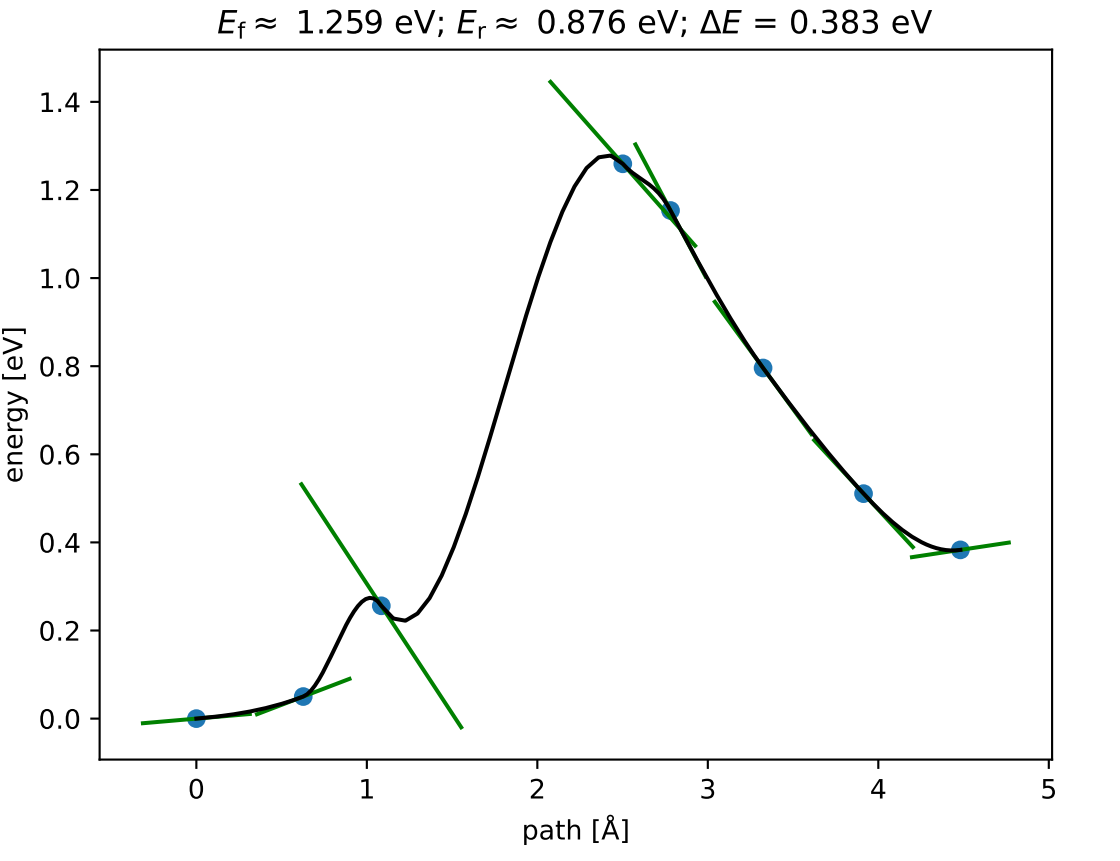
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
1
2
3
4


$E_f \approx$ 1.259 eV; $E_r \approx$ 0.876 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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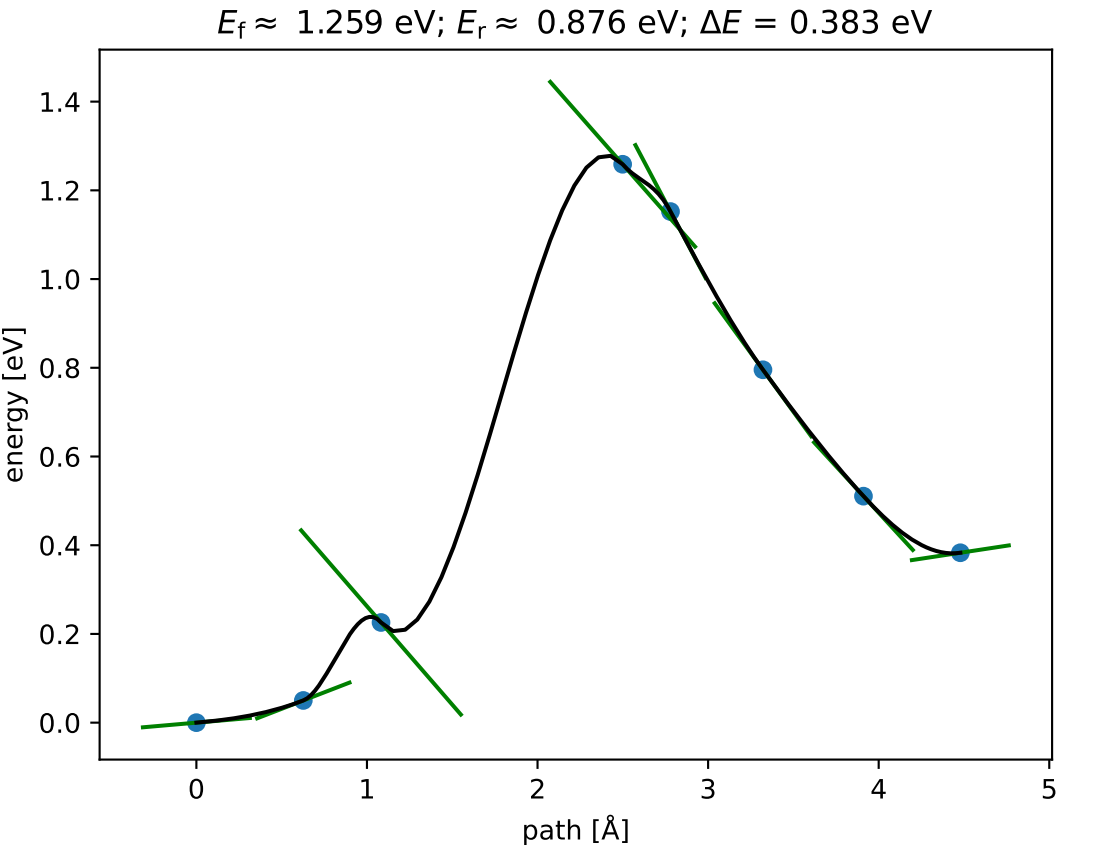
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.259 eV; $E_r \approx$ 0.876 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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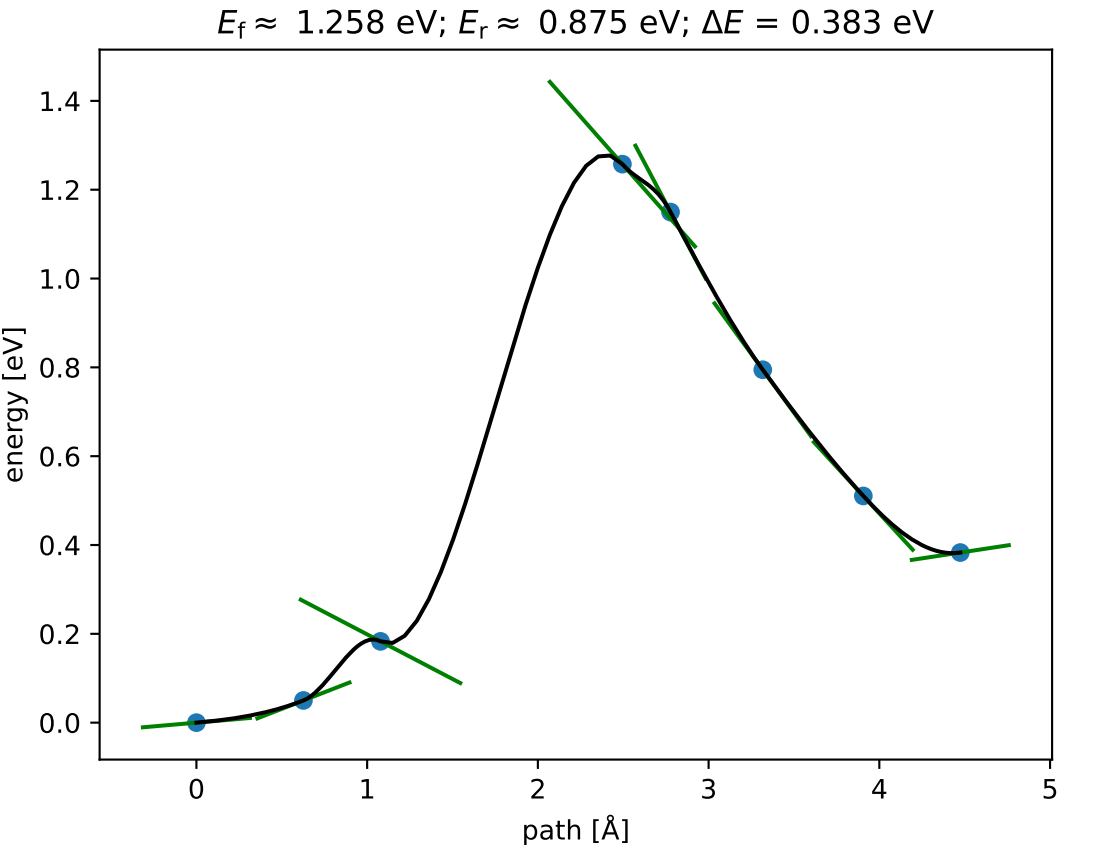
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.258 eV; $E_r \approx$ 0.875 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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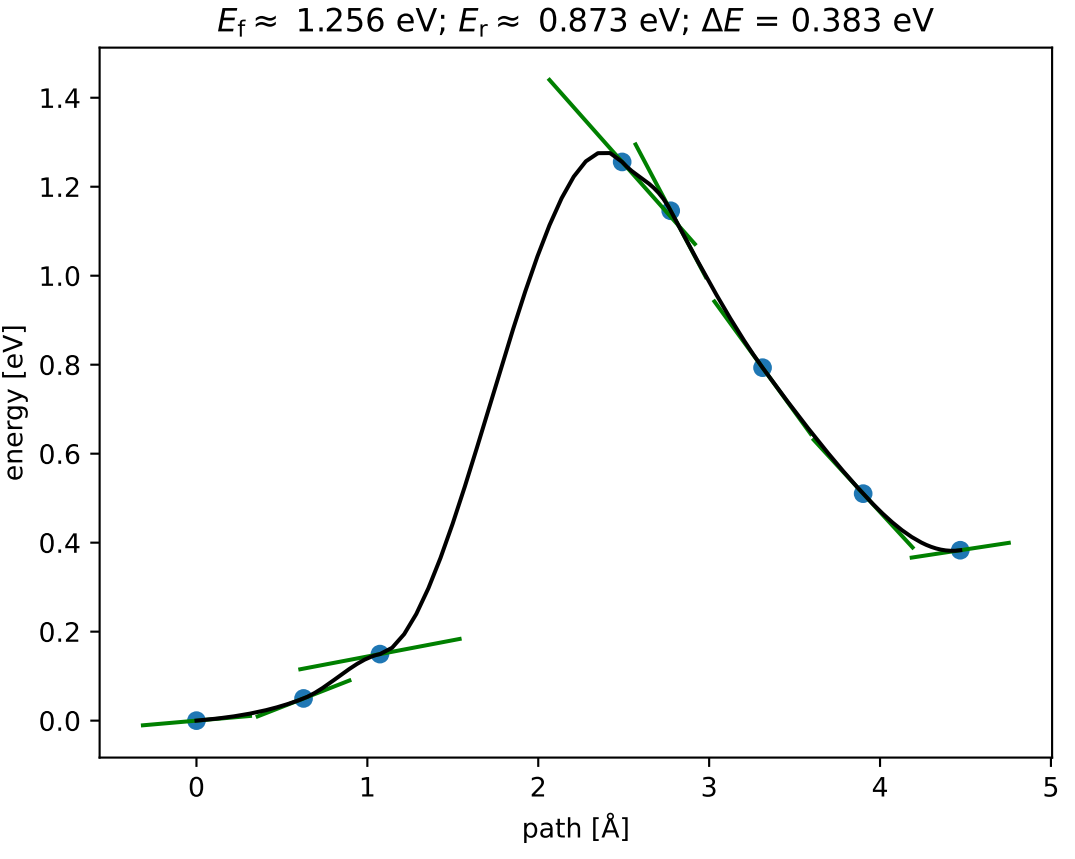
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.256 eV; $E_r \approx$ 0.873 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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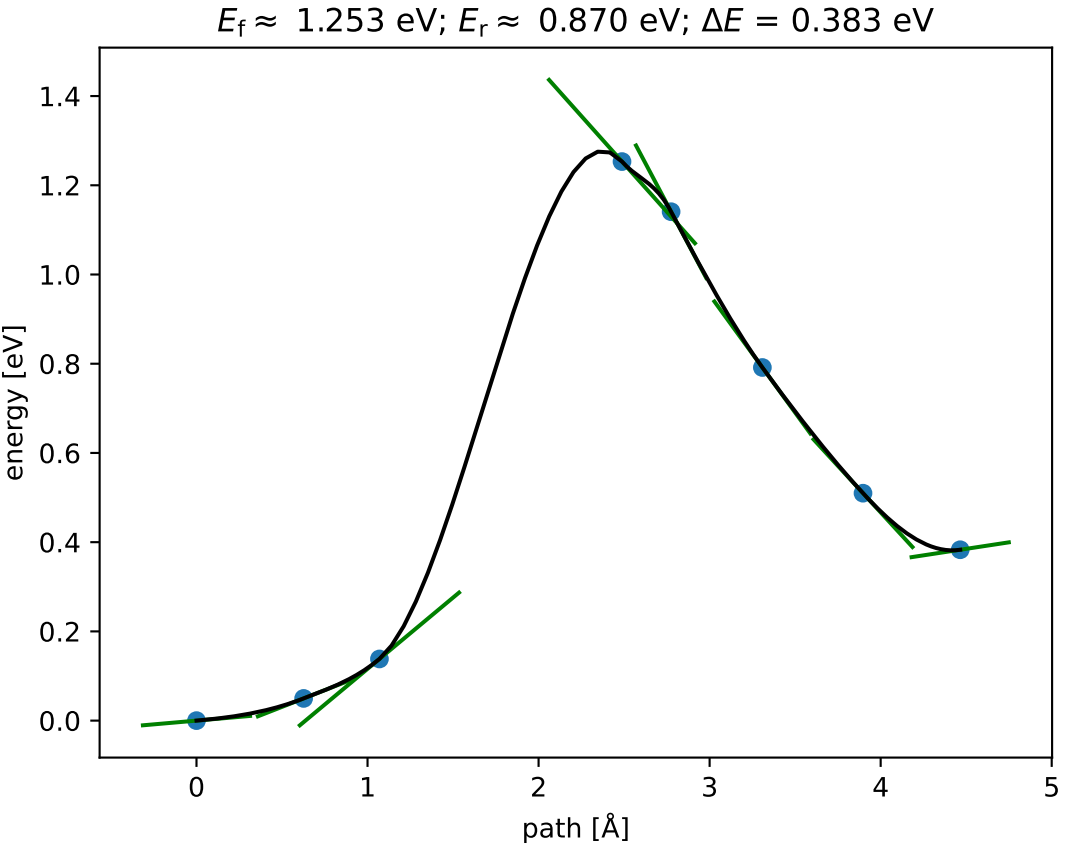
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.253 eV; $E_r \approx$ 0.870 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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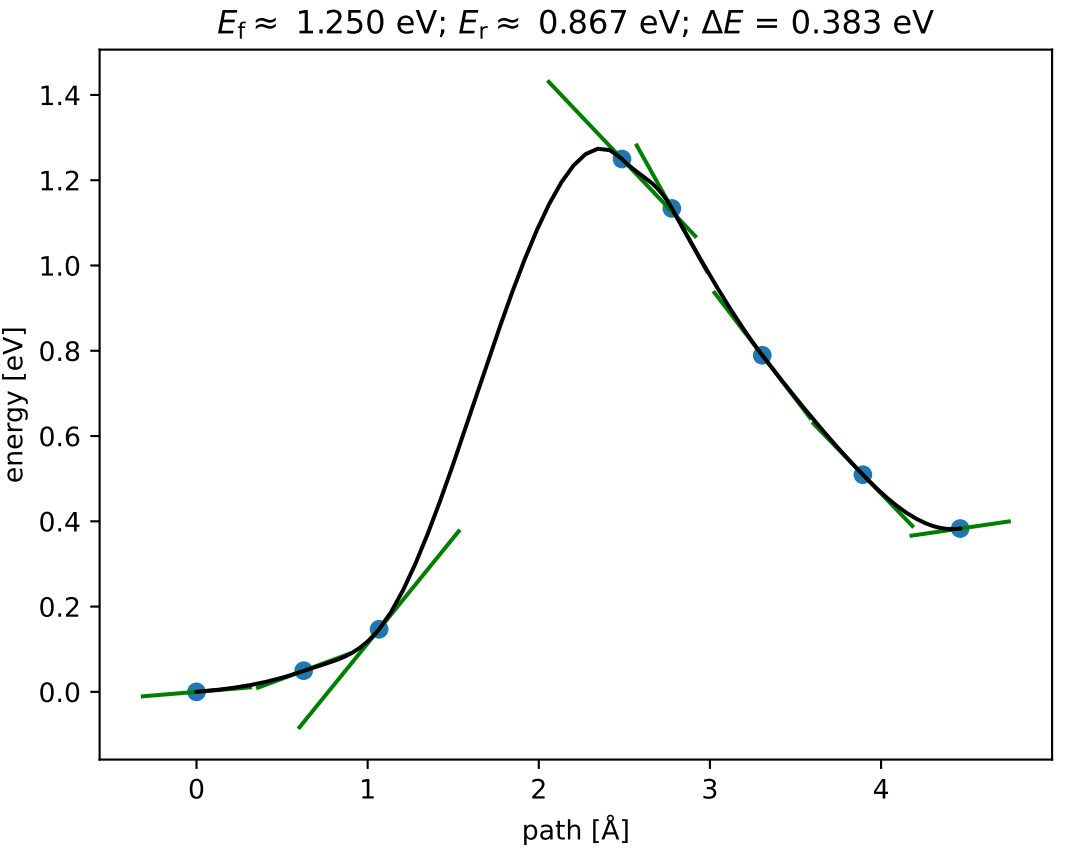
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.250 eV; $E_r \approx$ 0.867 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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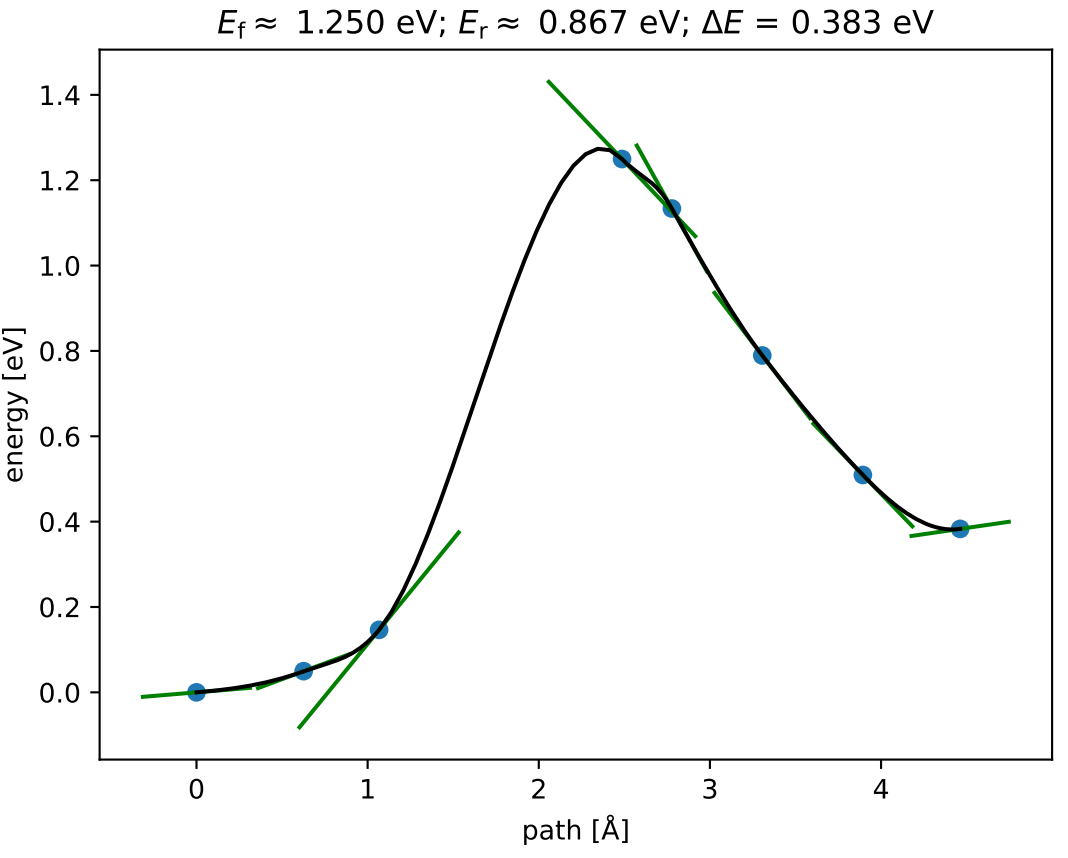
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4


$E_f \approx$ 1.250 eV; $E_r \approx$ 0.867 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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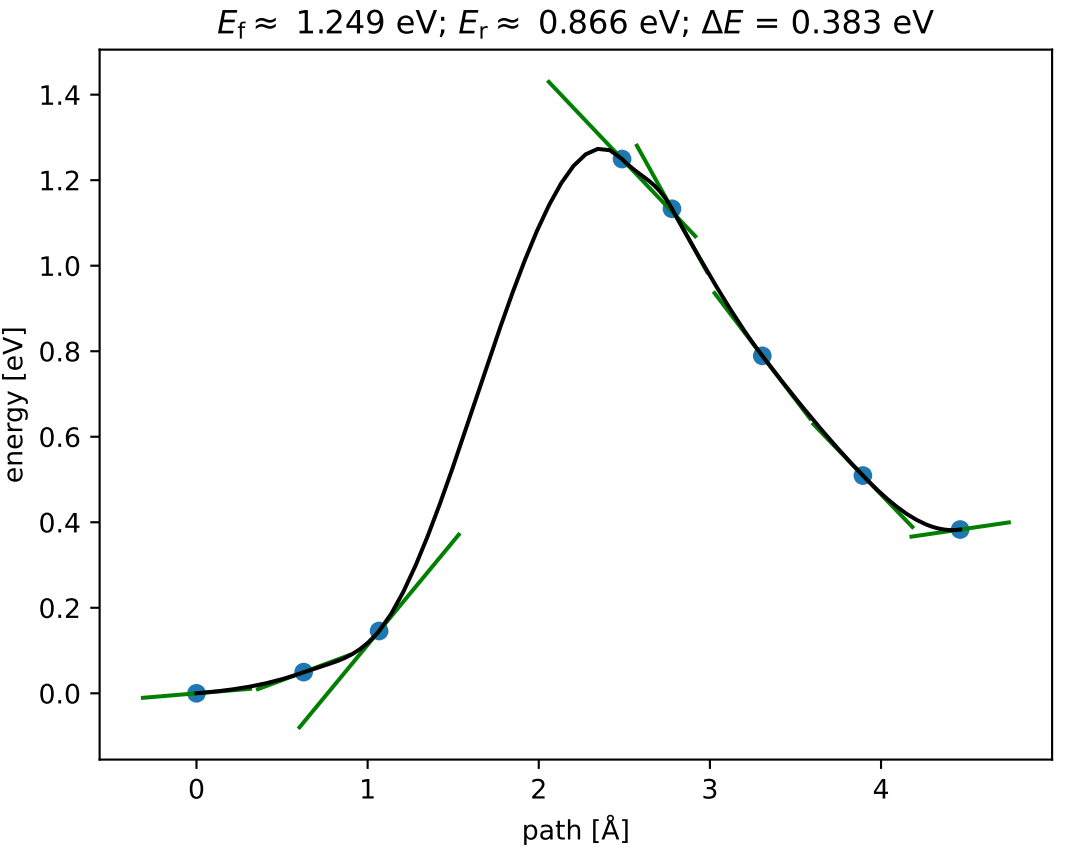
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4


$E_f \approx$ 1.249 eV; $E_r \approx$ 0.866 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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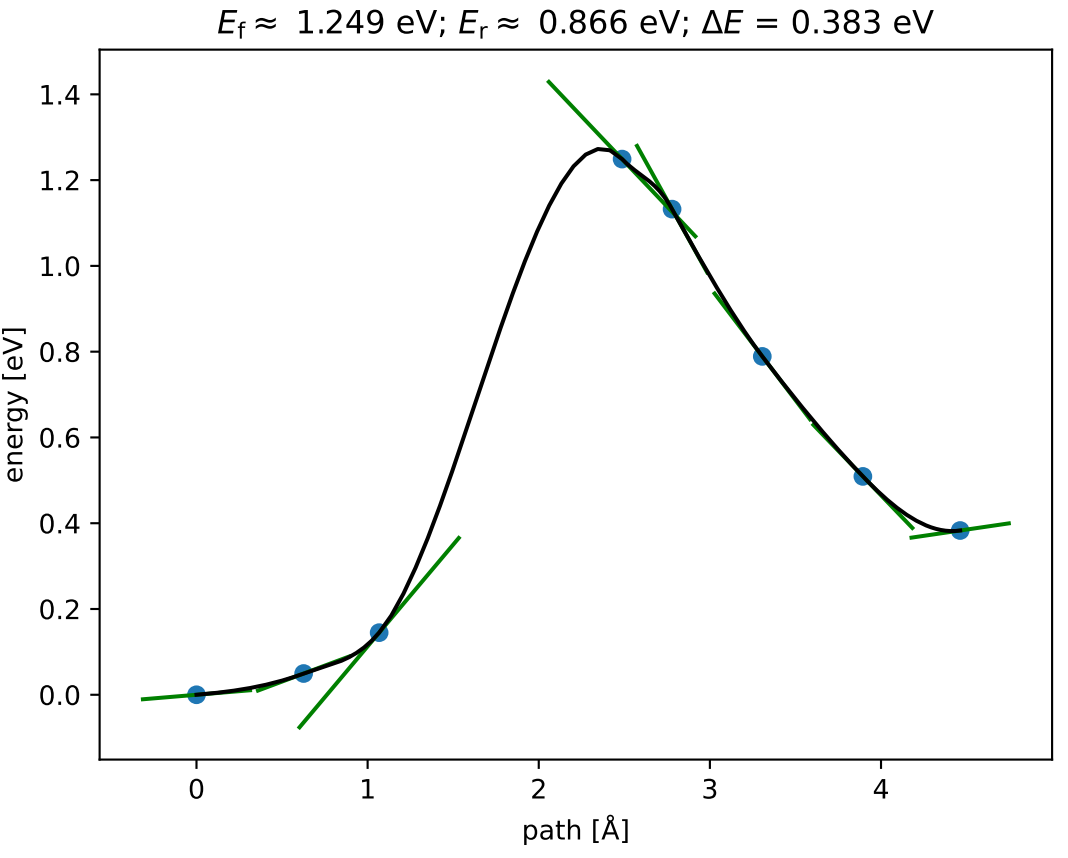
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4


$E_f \approx$ 1.249 eV; $E_r \approx$ 0.866 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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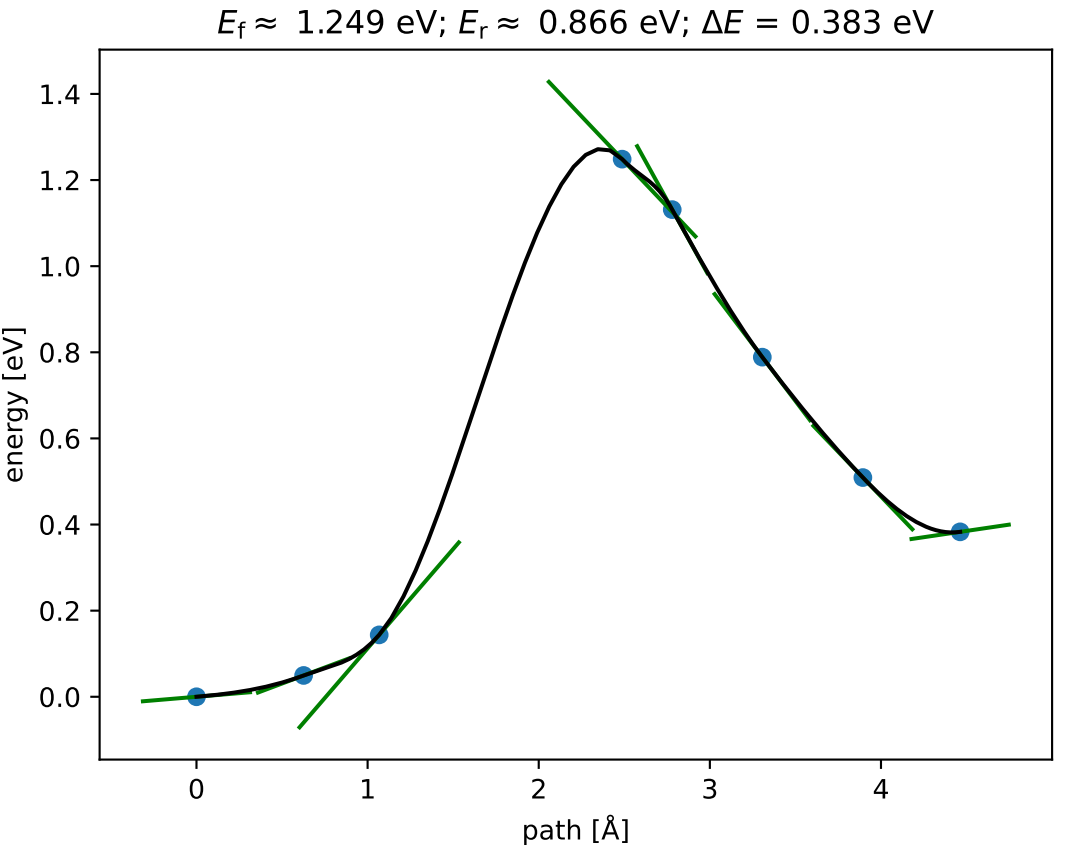
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4


$E_f \approx$ 1.249 eV; $E_r \approx$ 0.866 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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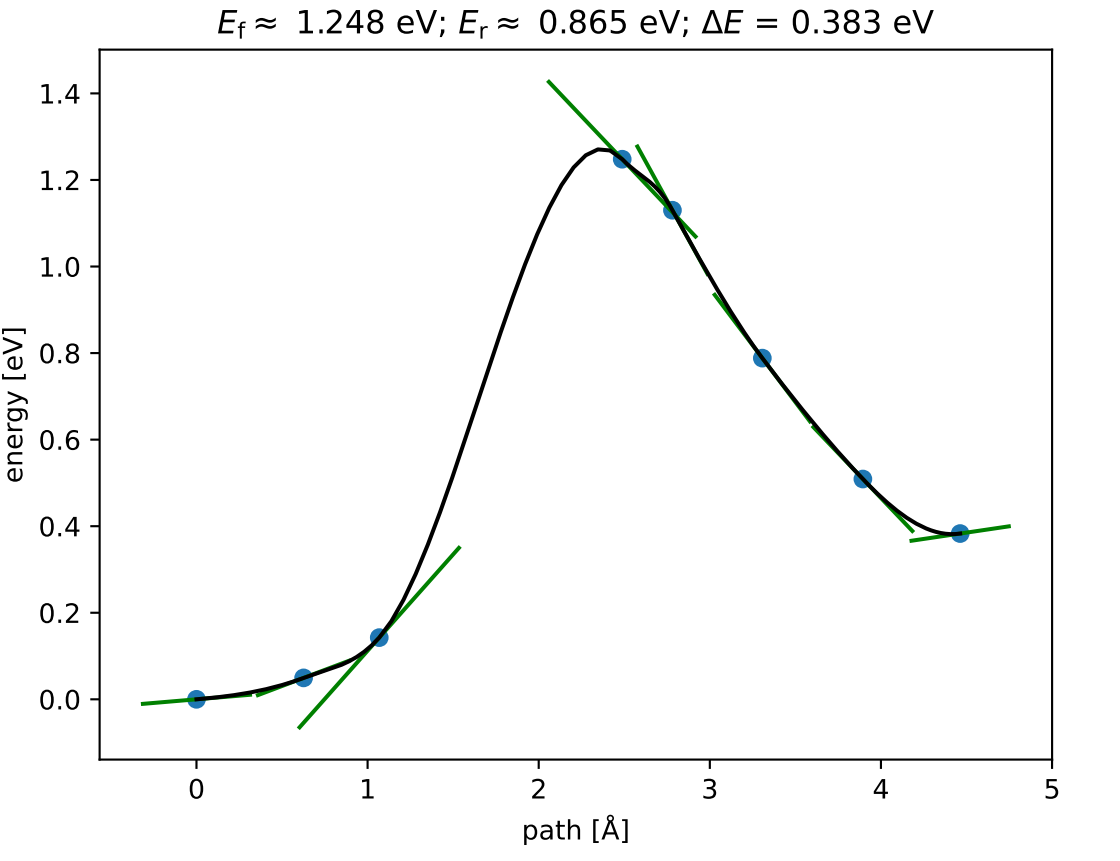
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4


$E_f \approx$ 1.248 eV; $E_r \approx$ 0.865 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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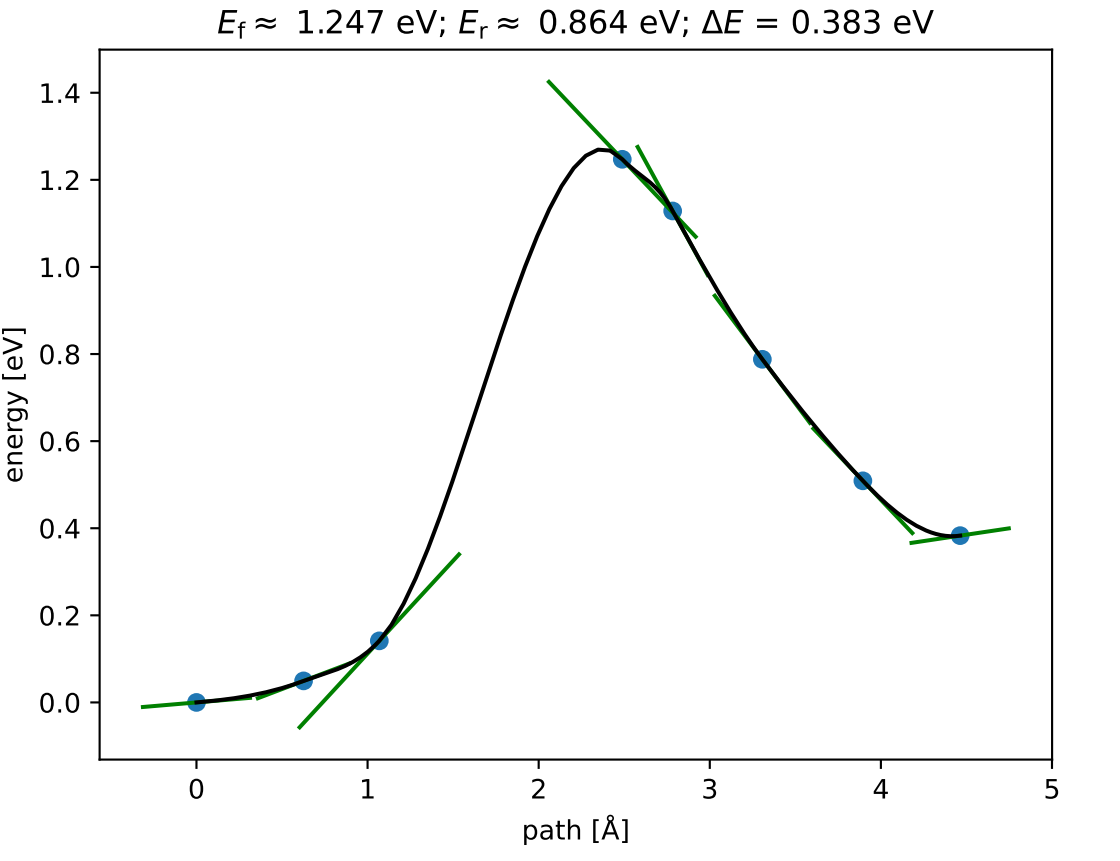
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.247 eV; $E_r \approx$ 0.864 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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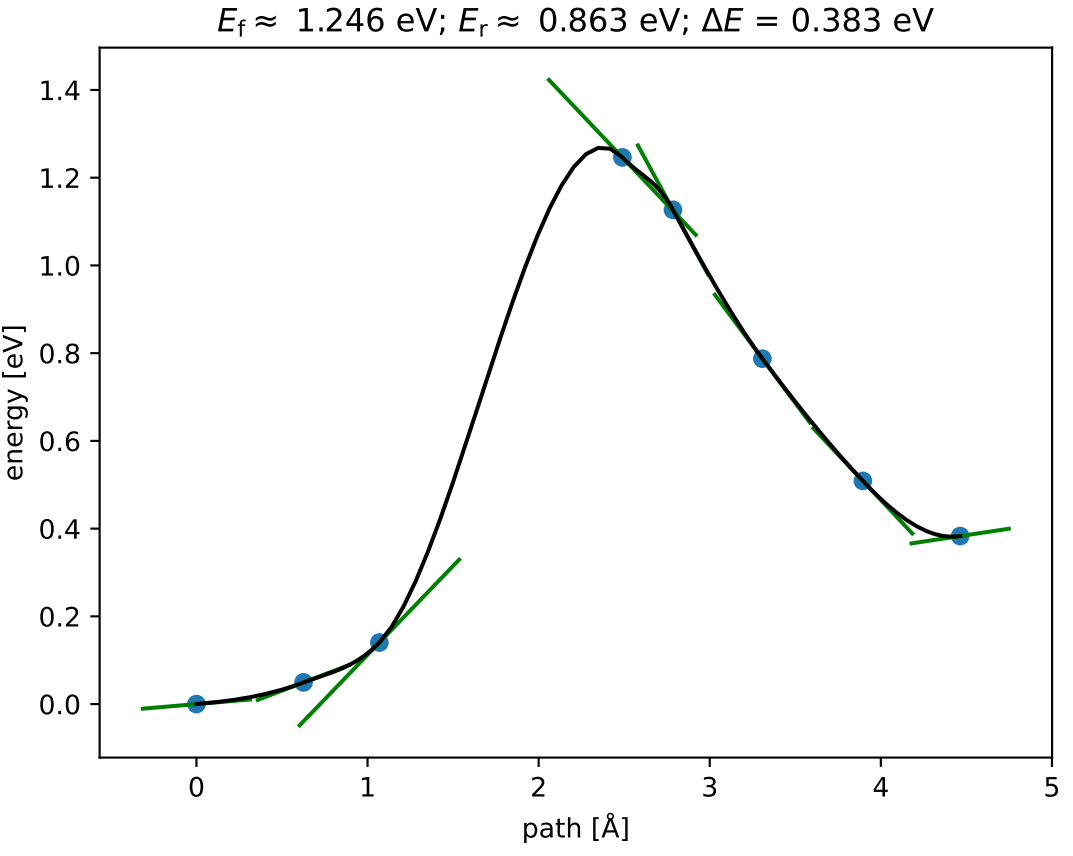
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.246 eV; $E_r \approx$ 0.863 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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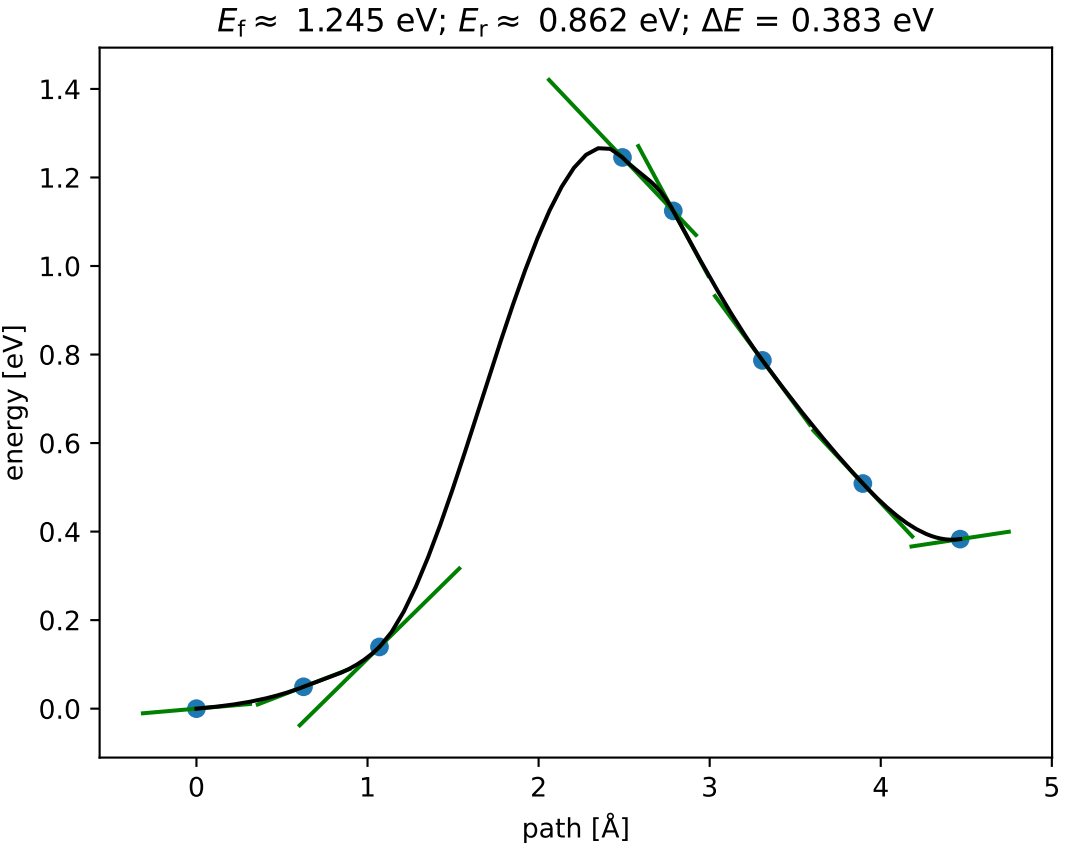
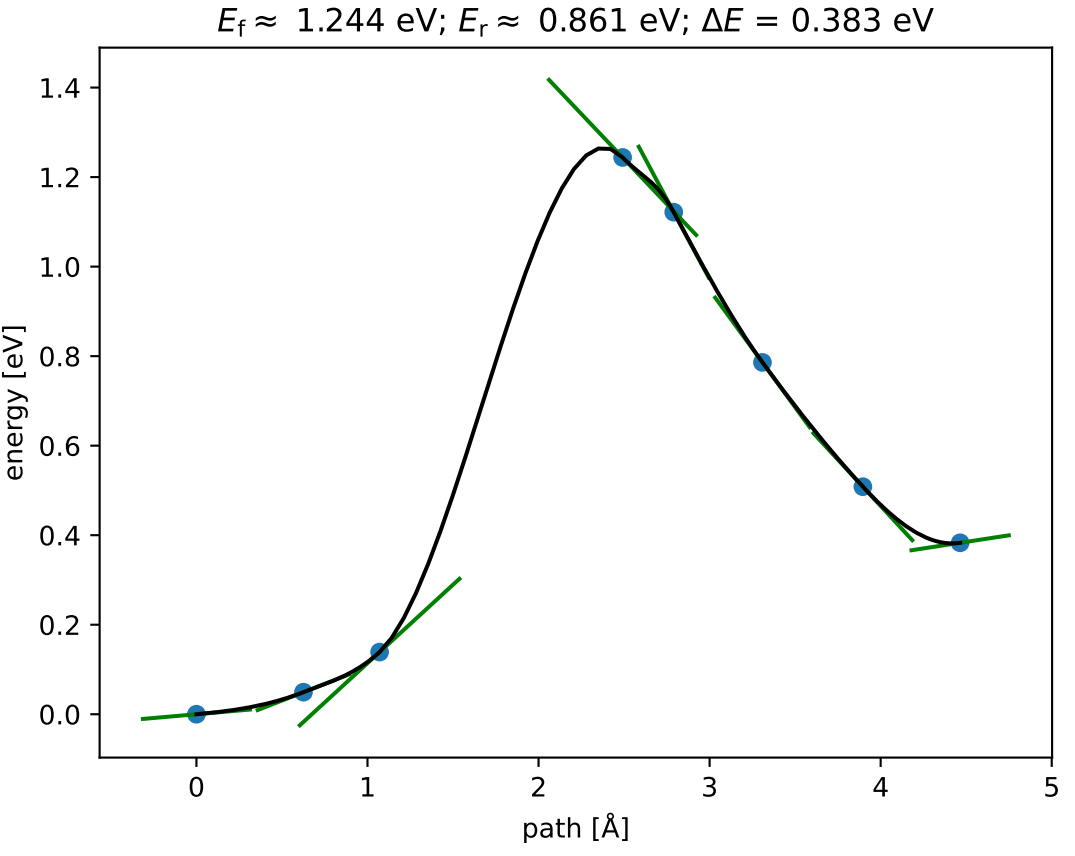
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.245 eV; $E_r \approx$ 0.862 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
5


$E_f \approx$ 1.244 eV; $E_r \approx$ 0.861 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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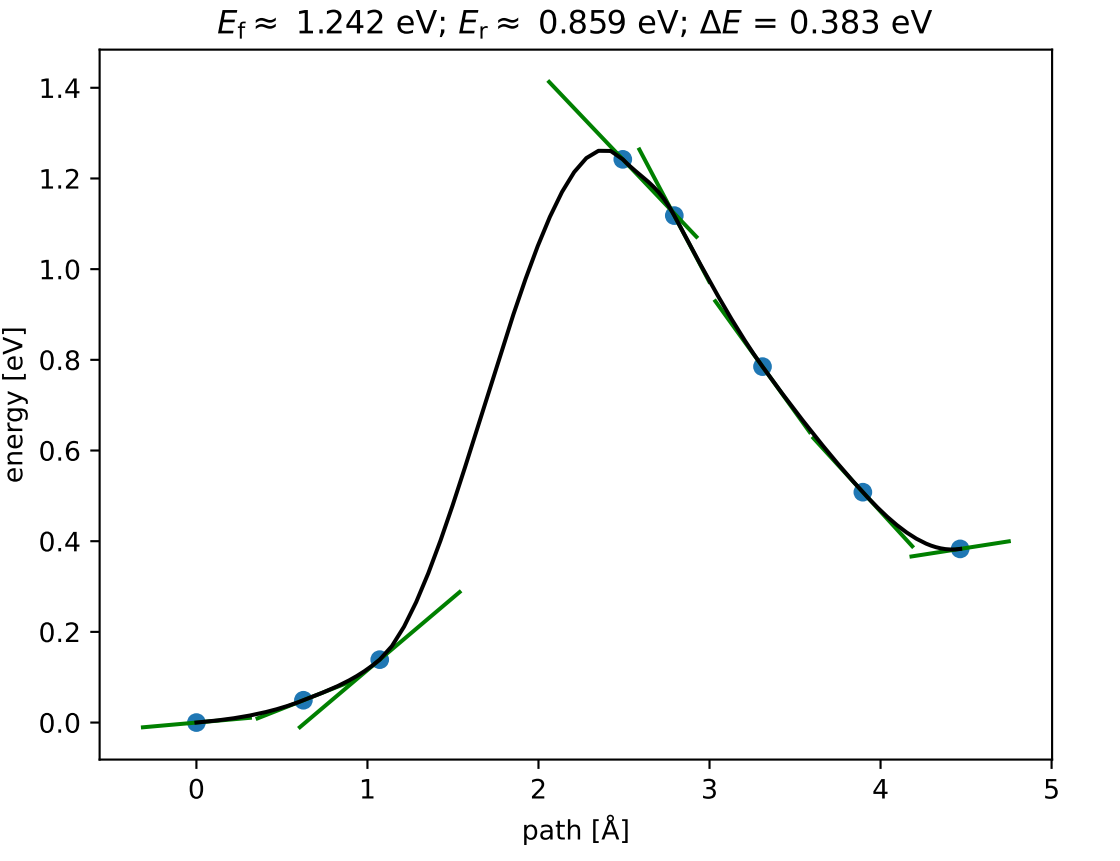
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.242 eV; $E_r \approx$ 0.859 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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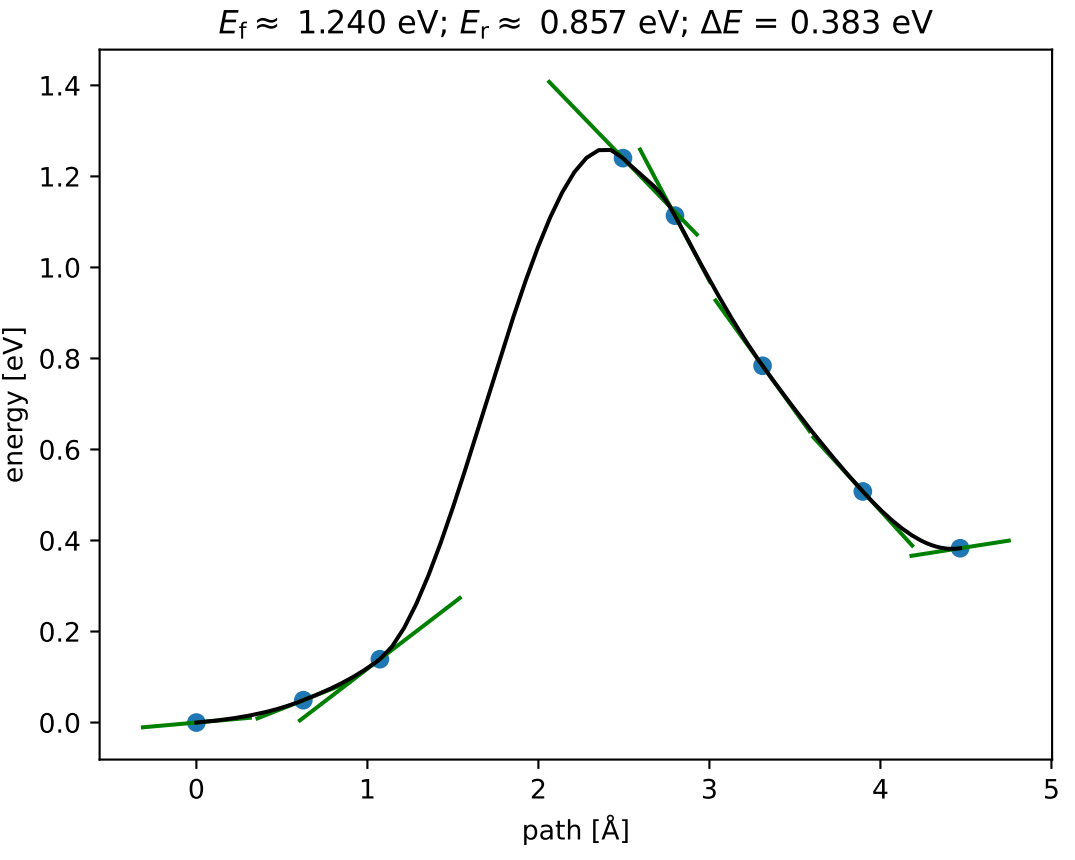
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.240 eV; $E_r \approx$ 0.857 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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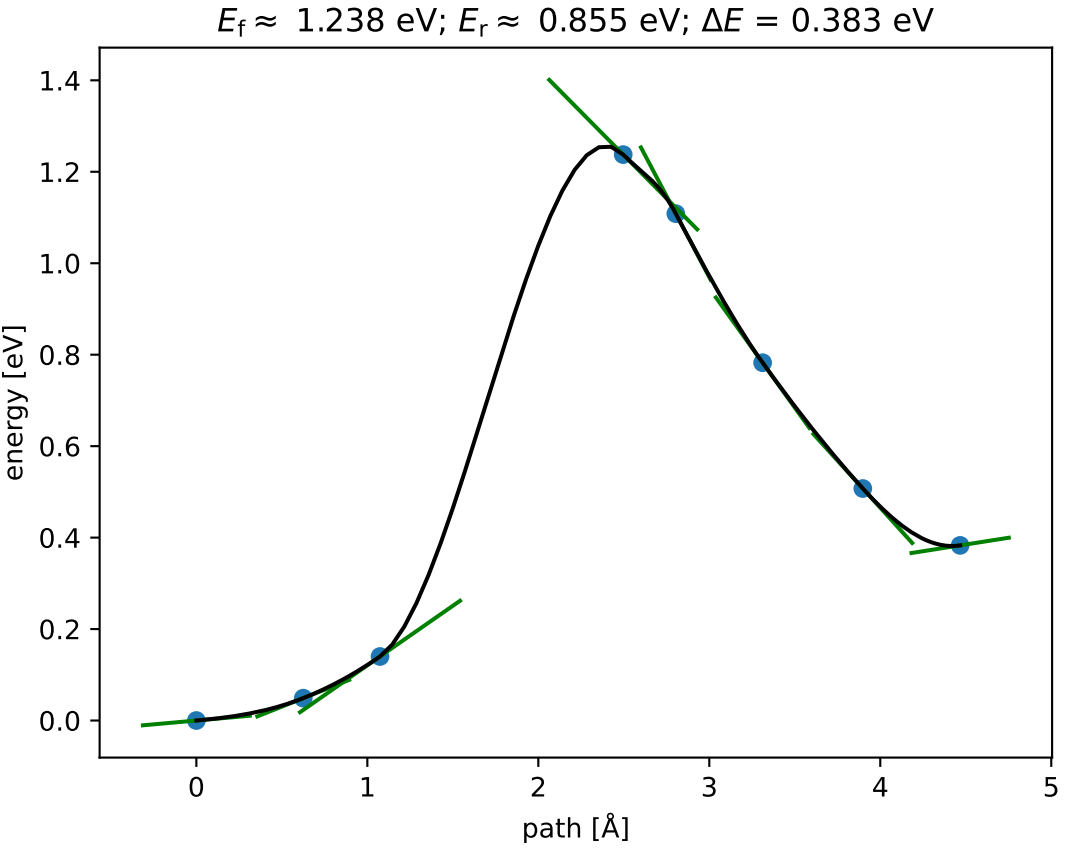
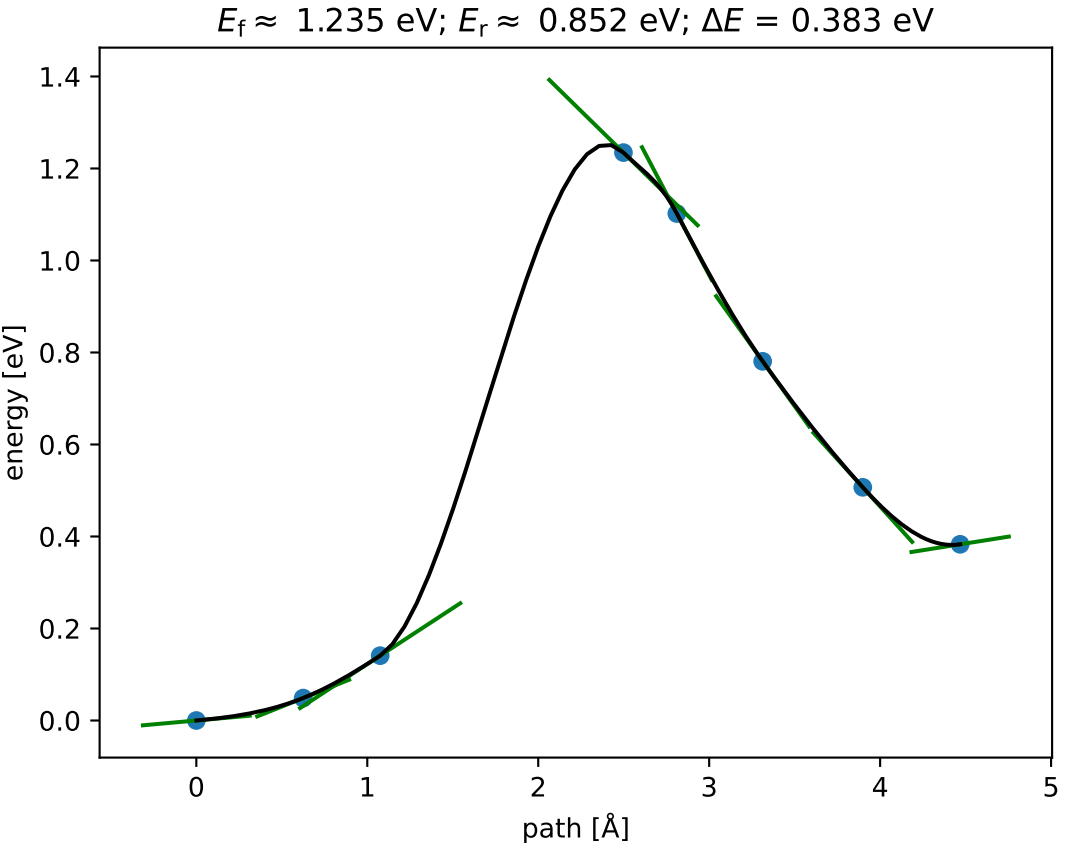
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 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
1.4
0
1
2
3
4
5


$E_f \approx$ 1.235 eV; $E_r \approx$ 0.852 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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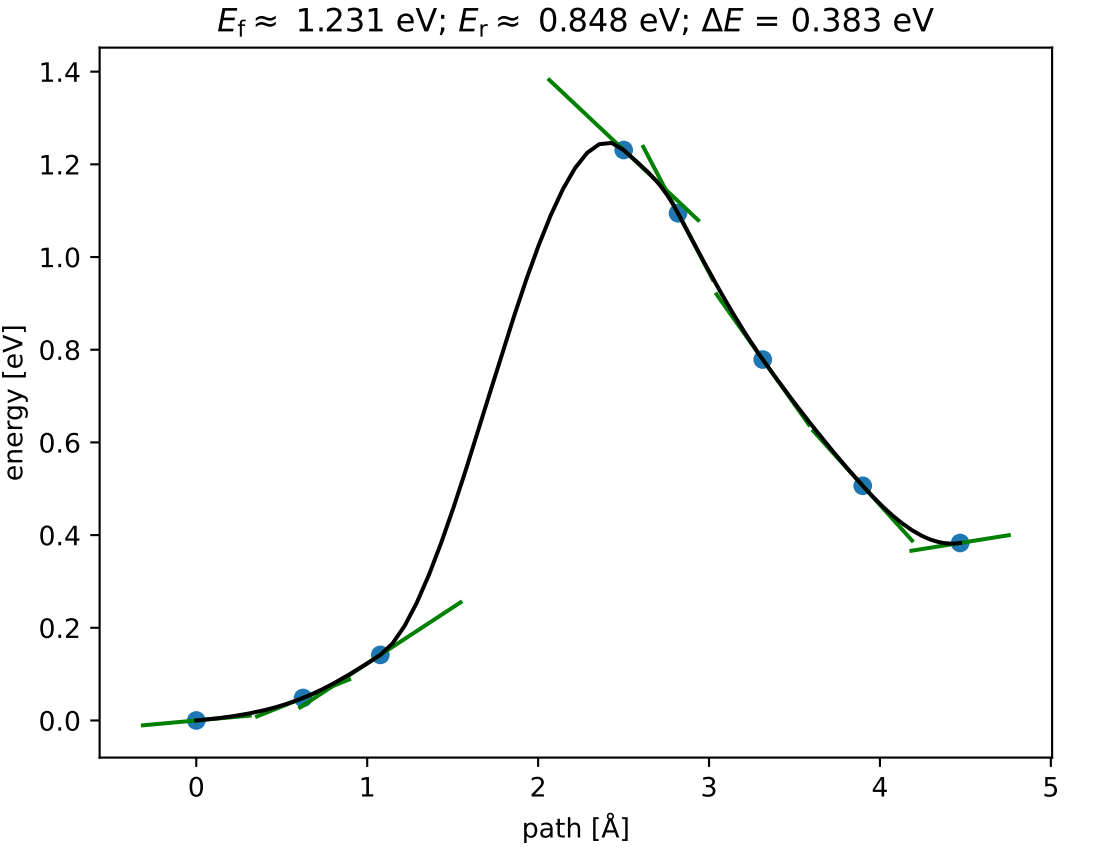
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.231 eV; $E_r \approx$ 0.848 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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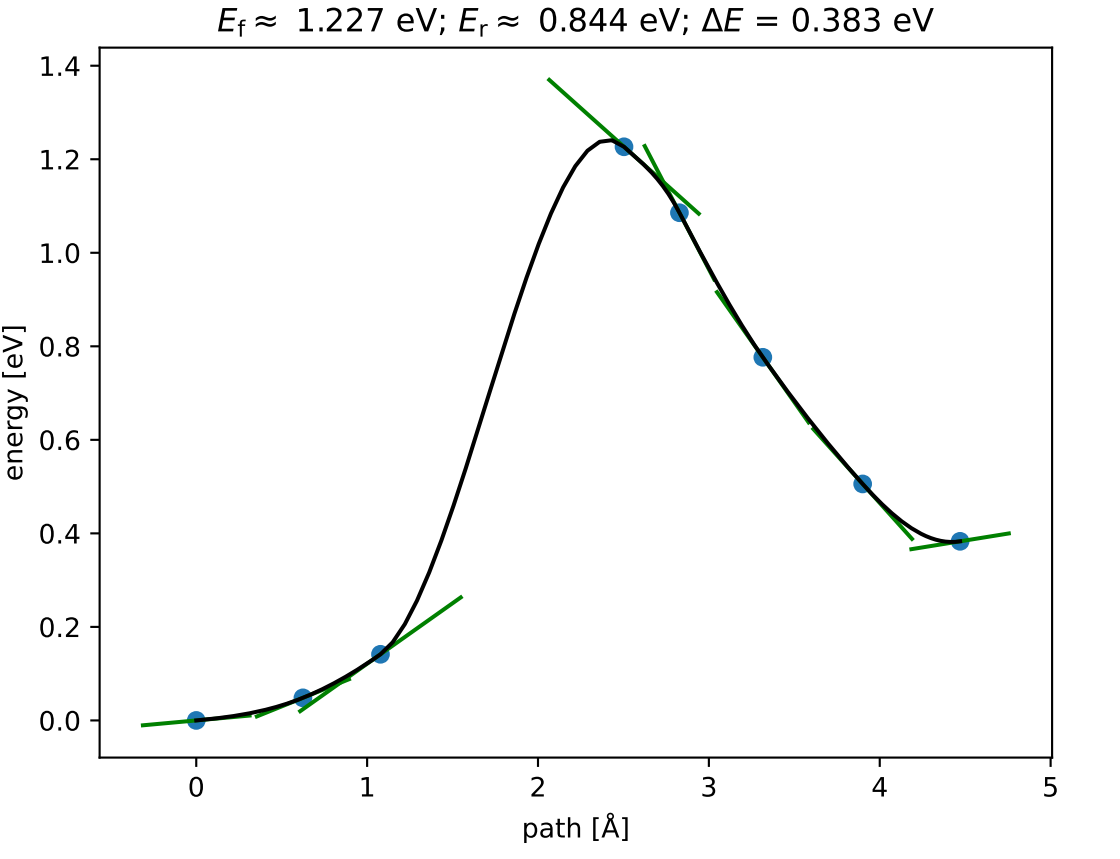
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.227 eV; $E_r \approx$ 0.844 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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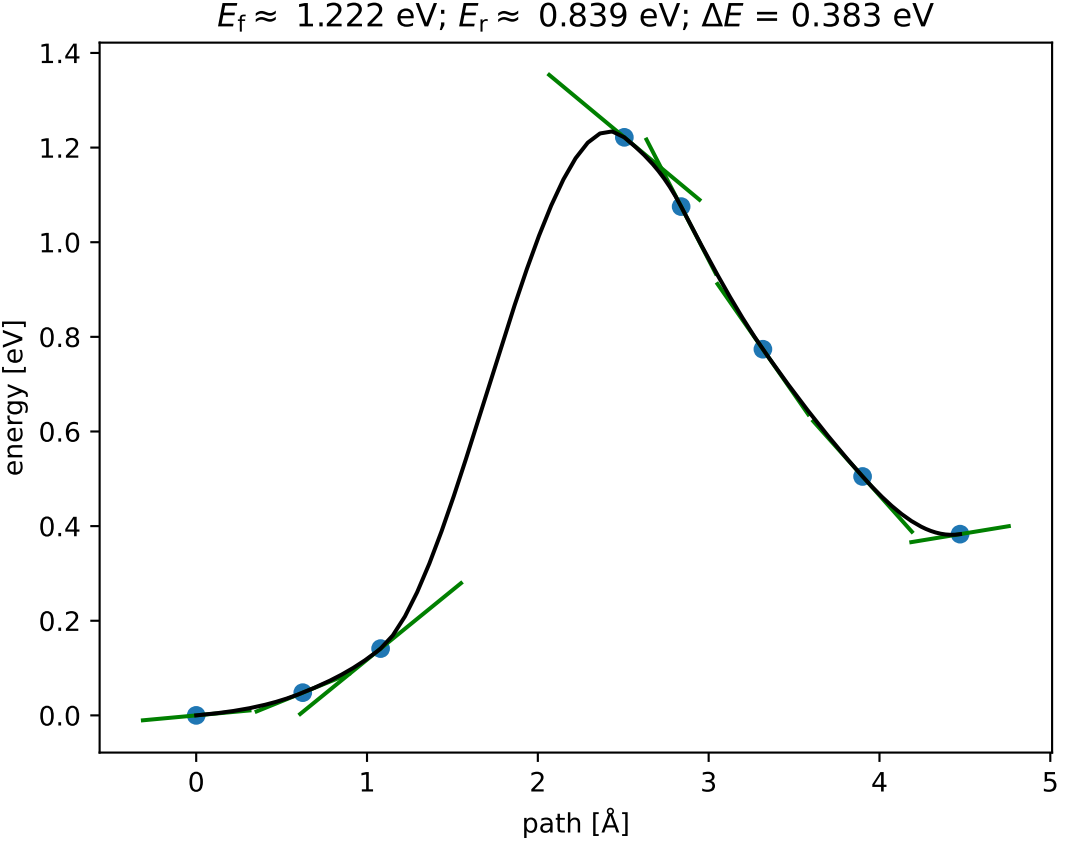
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.222 eV; $E_r \approx$ 0.839 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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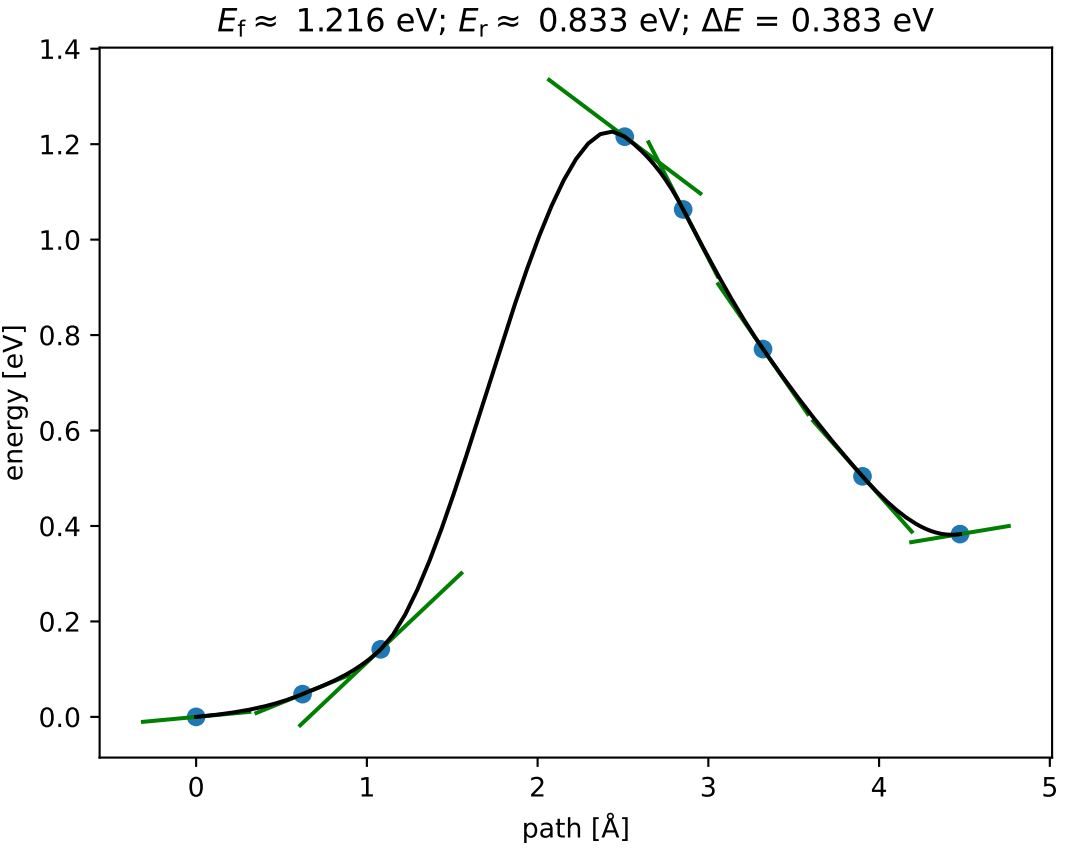
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.216 eV; $E_r \approx$ 0.833 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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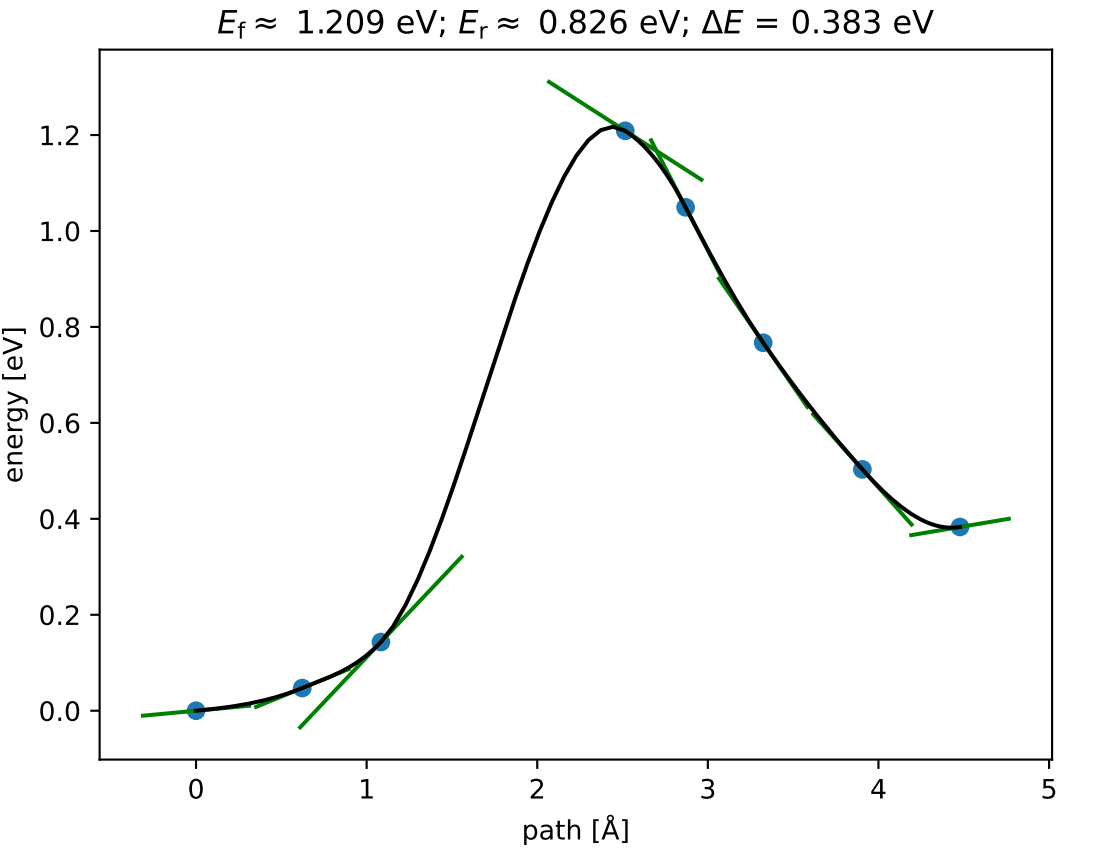
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.209 eV; $E_r \approx$ 0.826 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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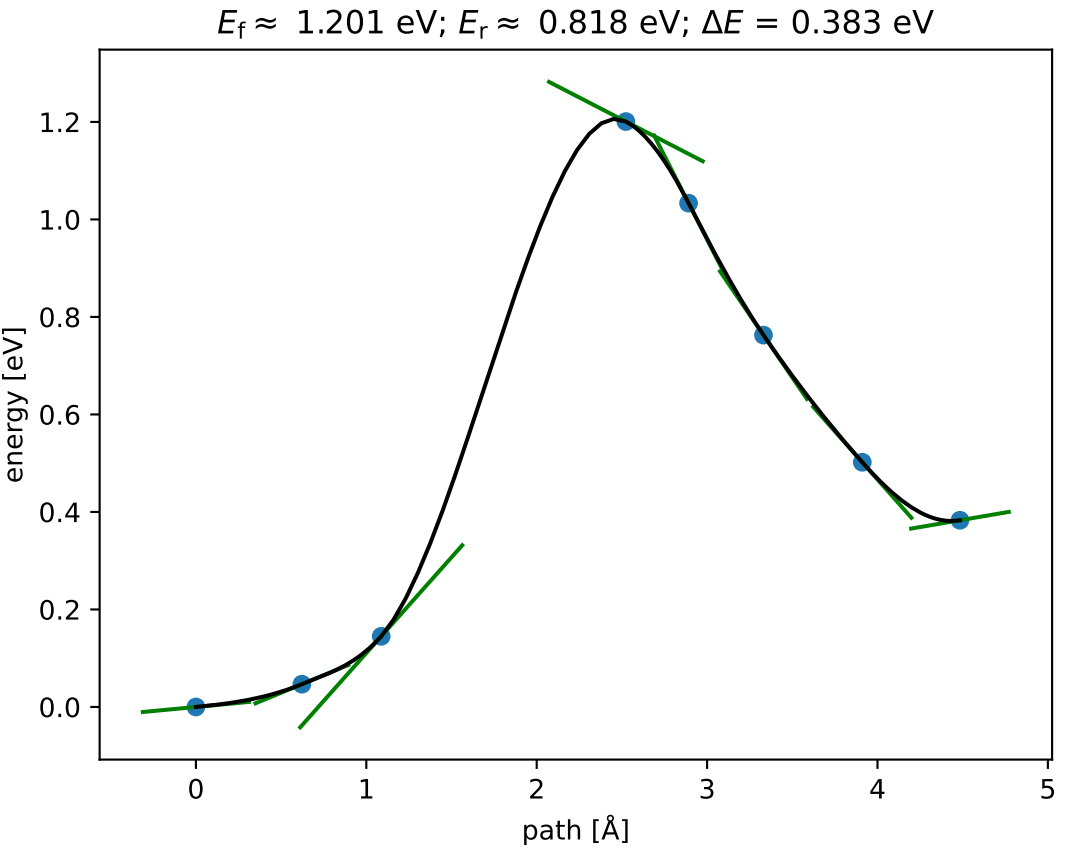
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.201 eV; $E_r \approx$ 0.818 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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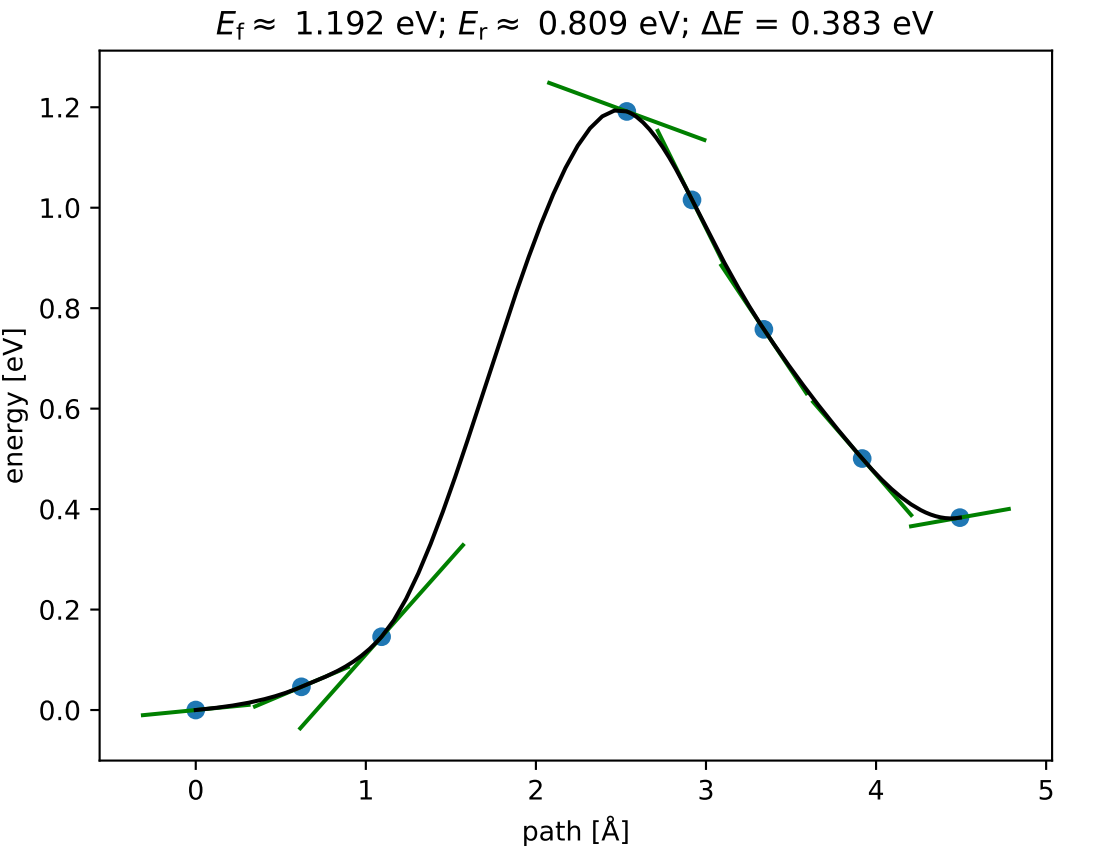
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.192 eV; $E_r \approx$ 0.809 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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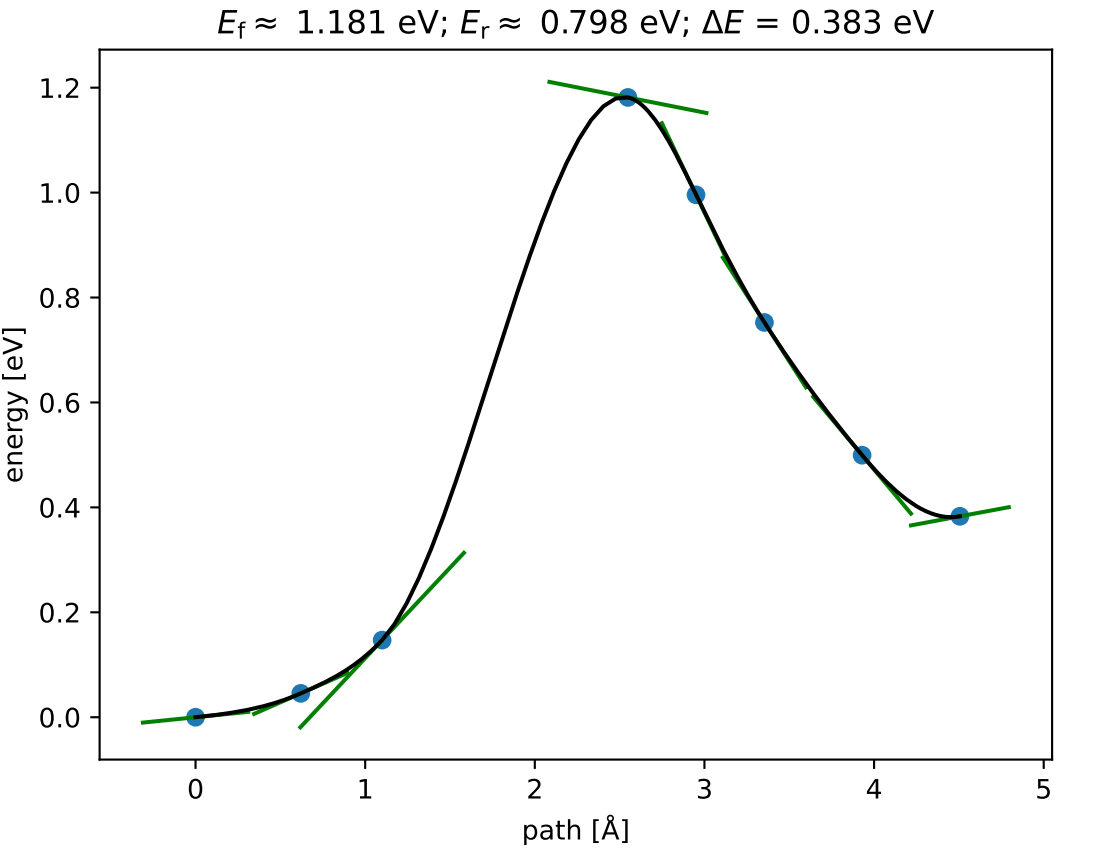
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.181 eV; $E_r \approx$ 0.798 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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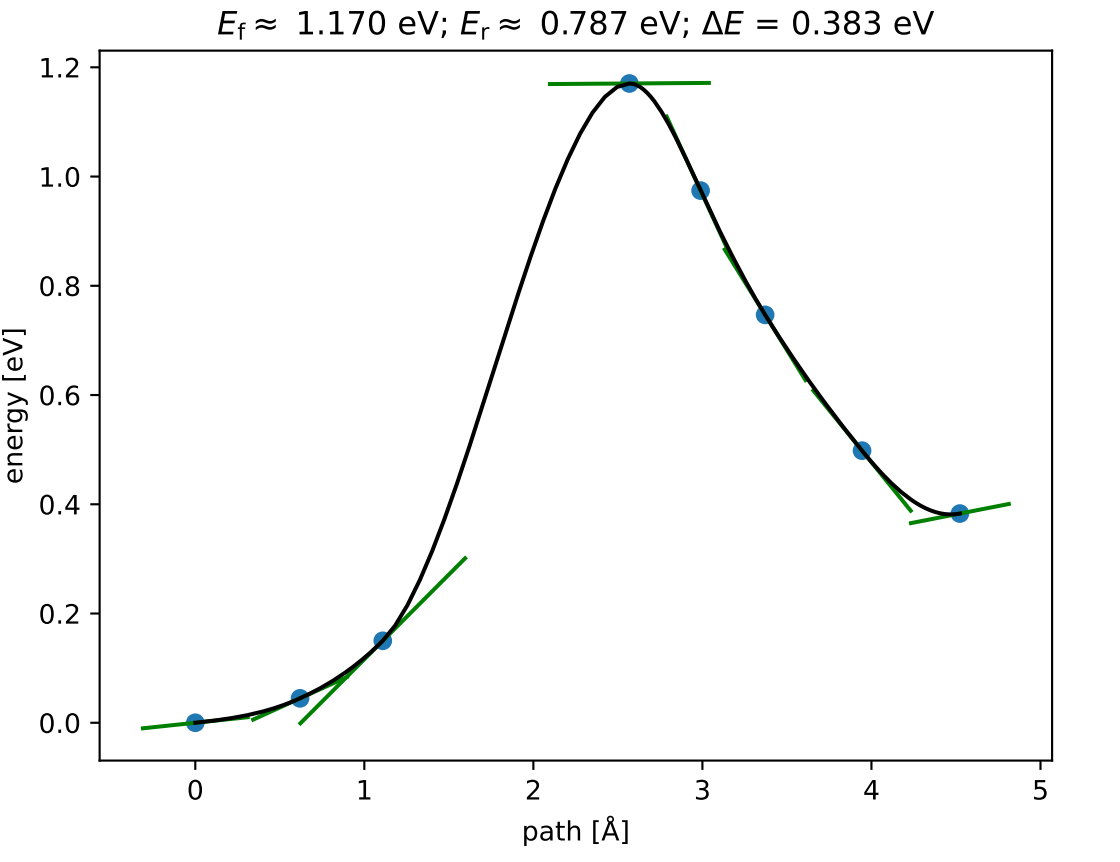
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.170 eV; $E_r \approx$ 0.787 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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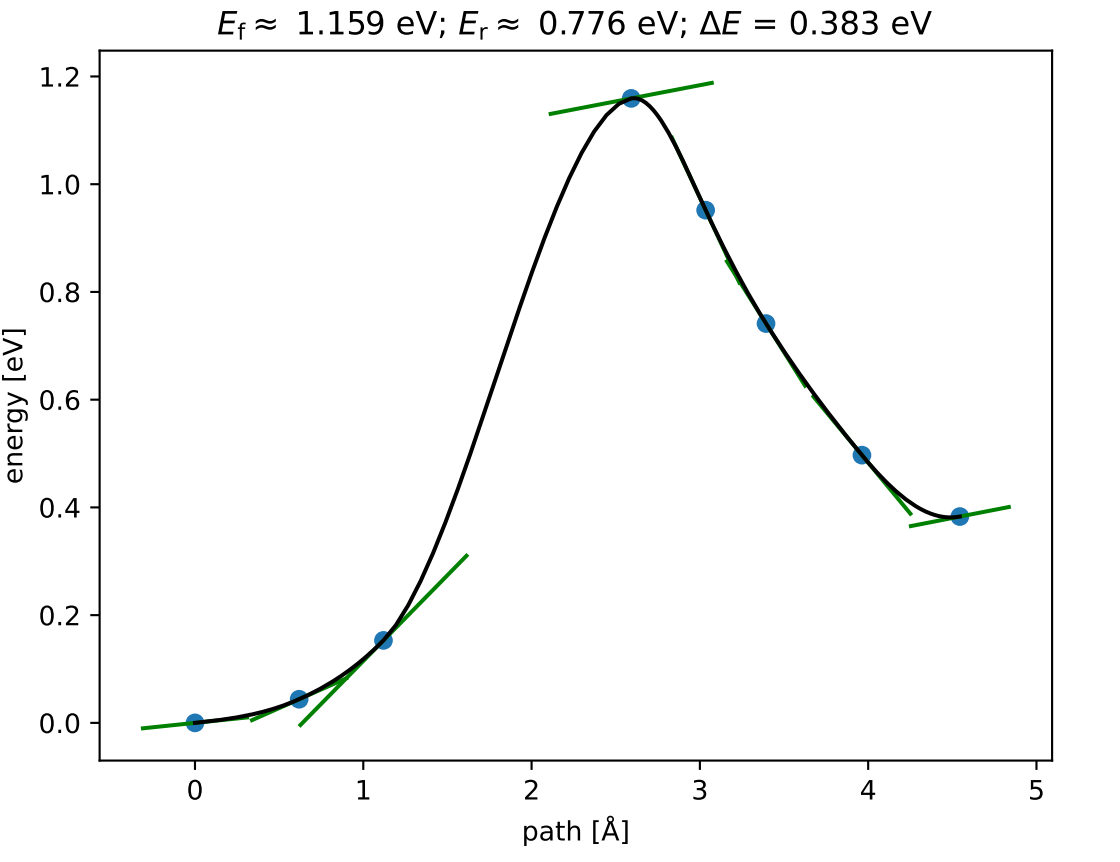
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.159 eV; $E_r \approx$ 0.776 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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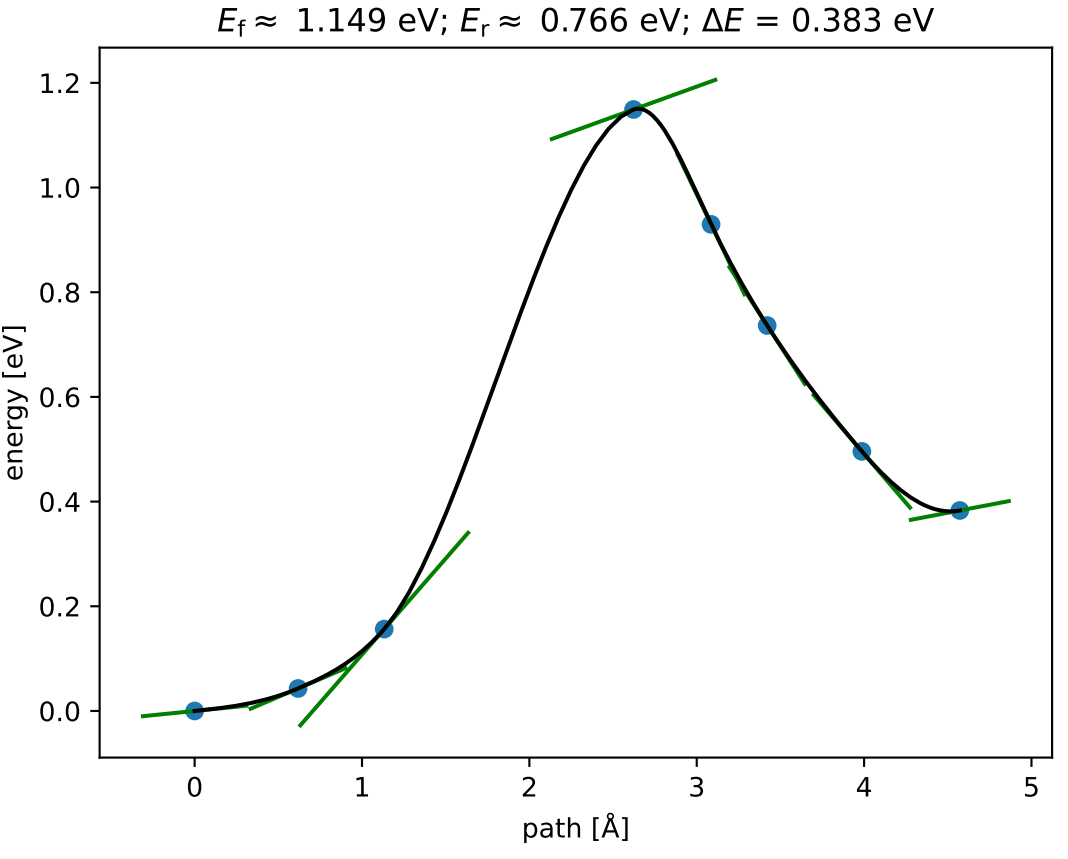
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.149 eV; $E_r \approx$ 0.766 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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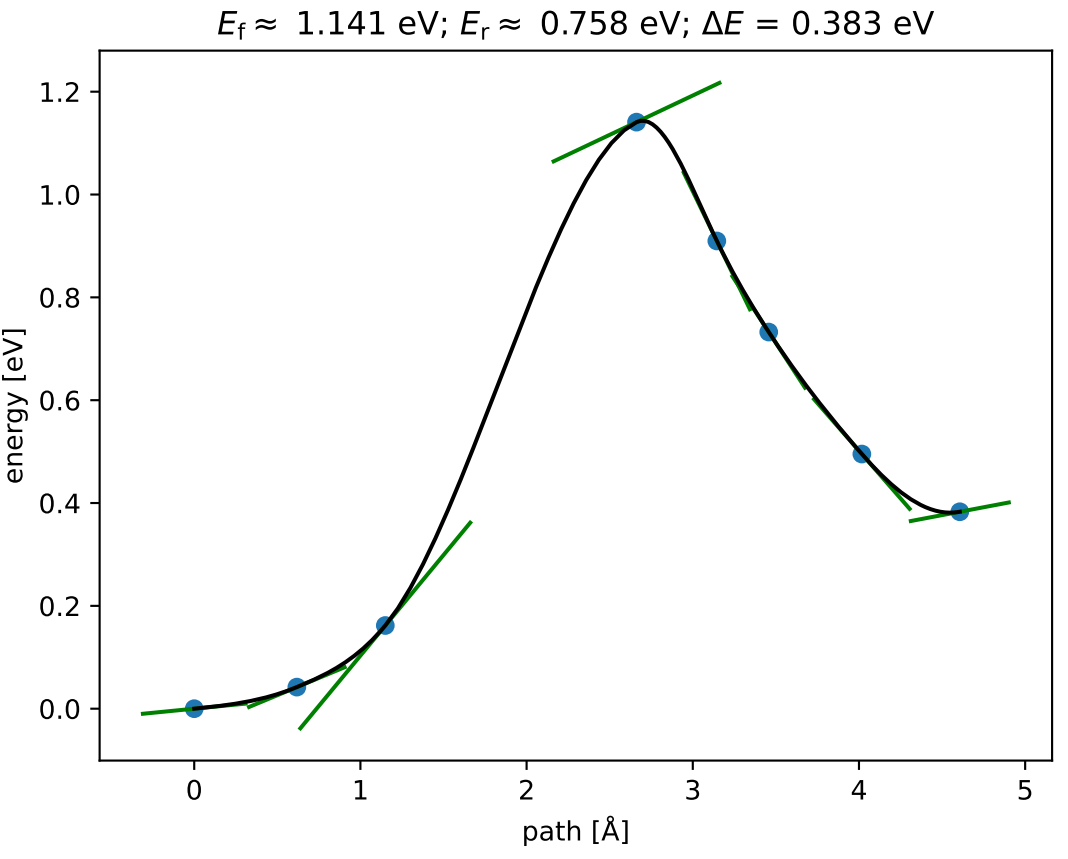
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.141 eV; $E_r \approx$ 0.758 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.2
0.4
0.6
0.8
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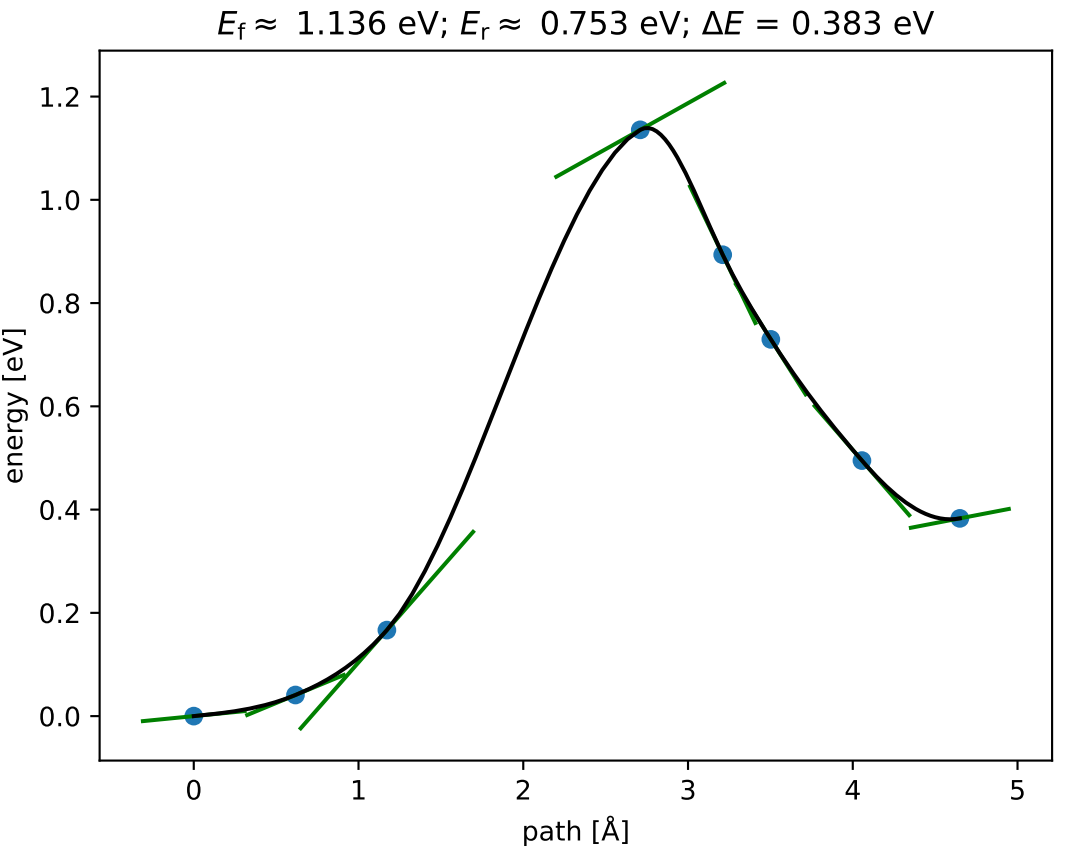
1.2
0
1
2
3
4
5


$E_f \approx$ 1.136 eV; $E_r \approx$ 0.753 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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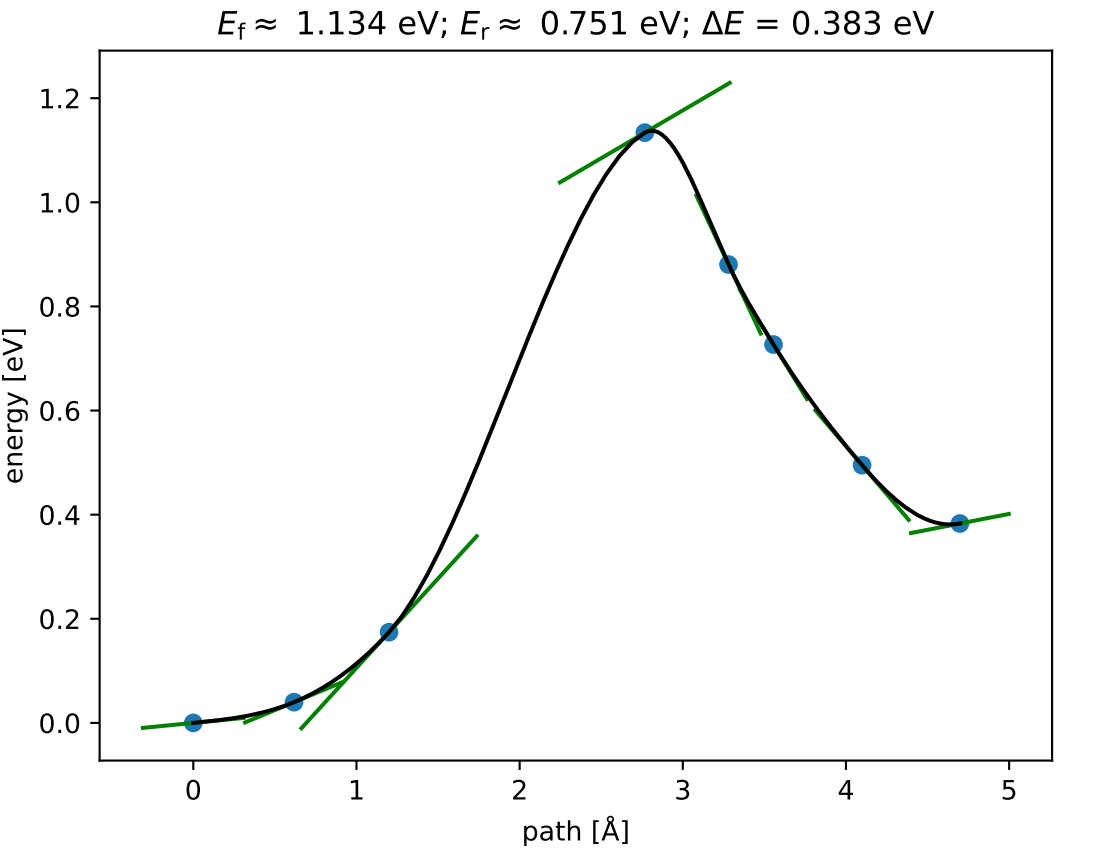
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.134 eV; $E_r \approx$ 0.751 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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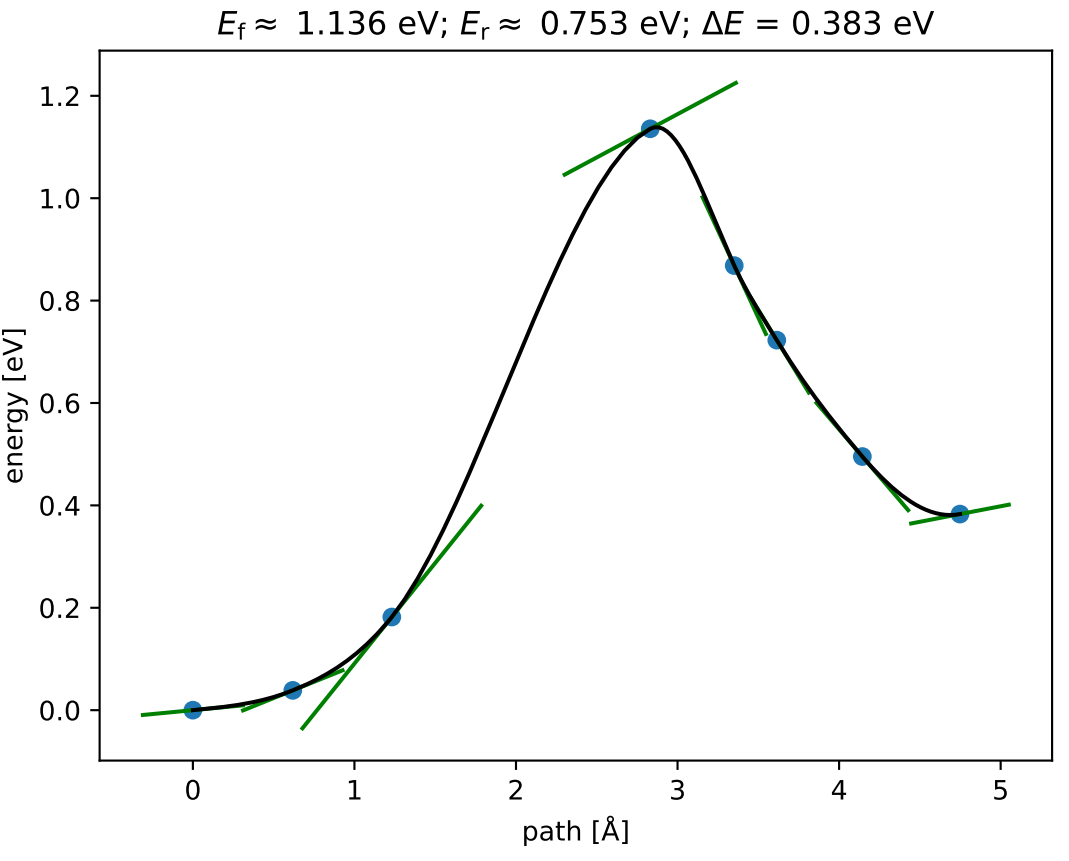
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.136 eV; $E_r \approx$ 0.753 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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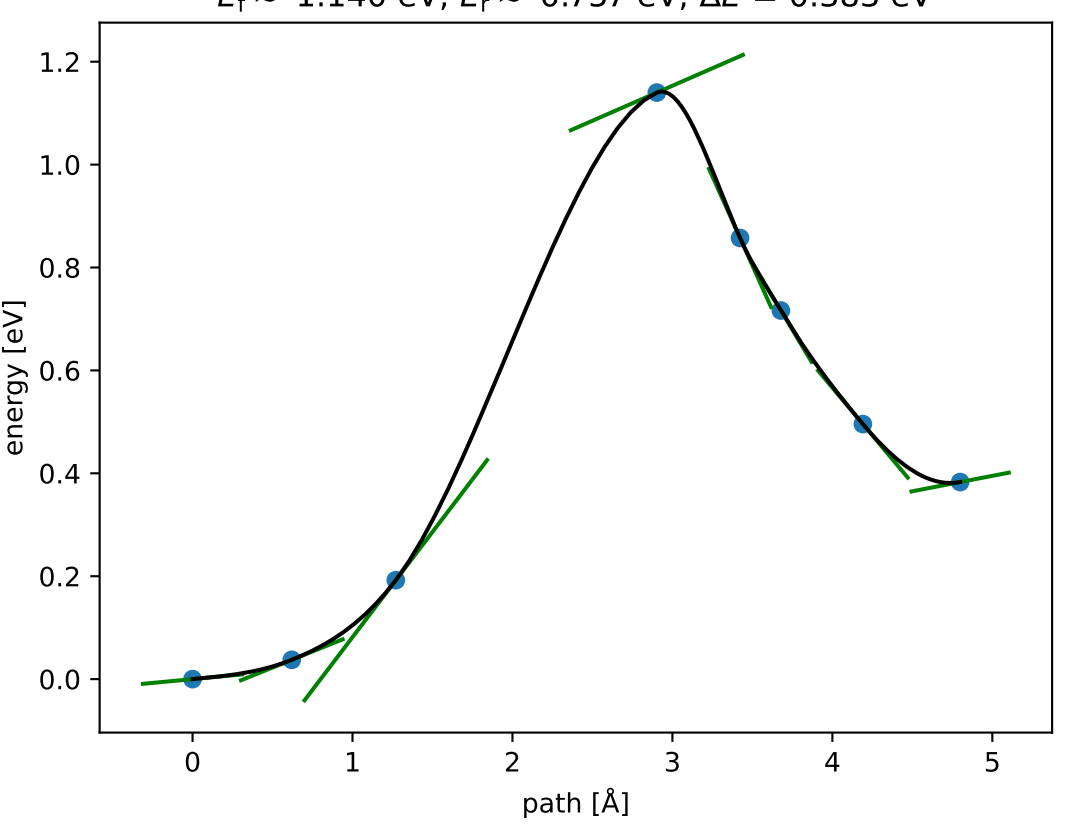
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.140 eV; $E_r \approx$ 0.757 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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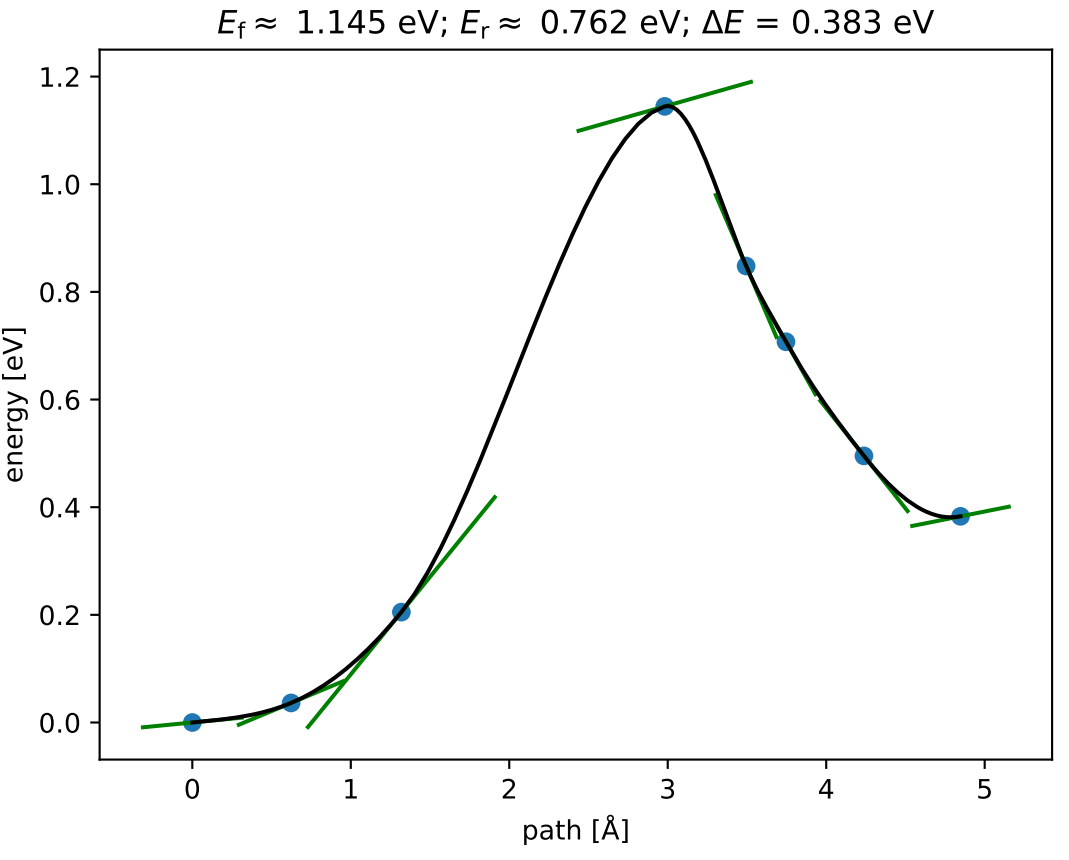
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.145 eV; $E_r \approx$ 0.762 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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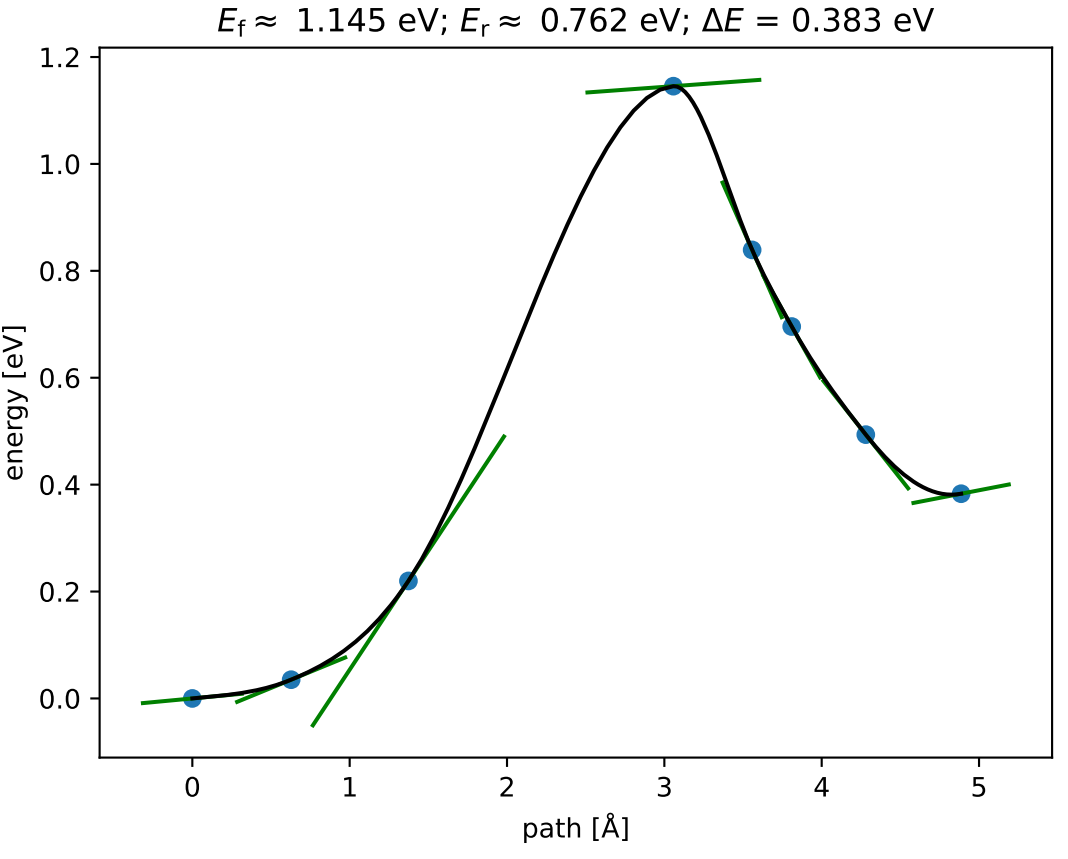
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.145 eV; $E_r \approx$ 0.762 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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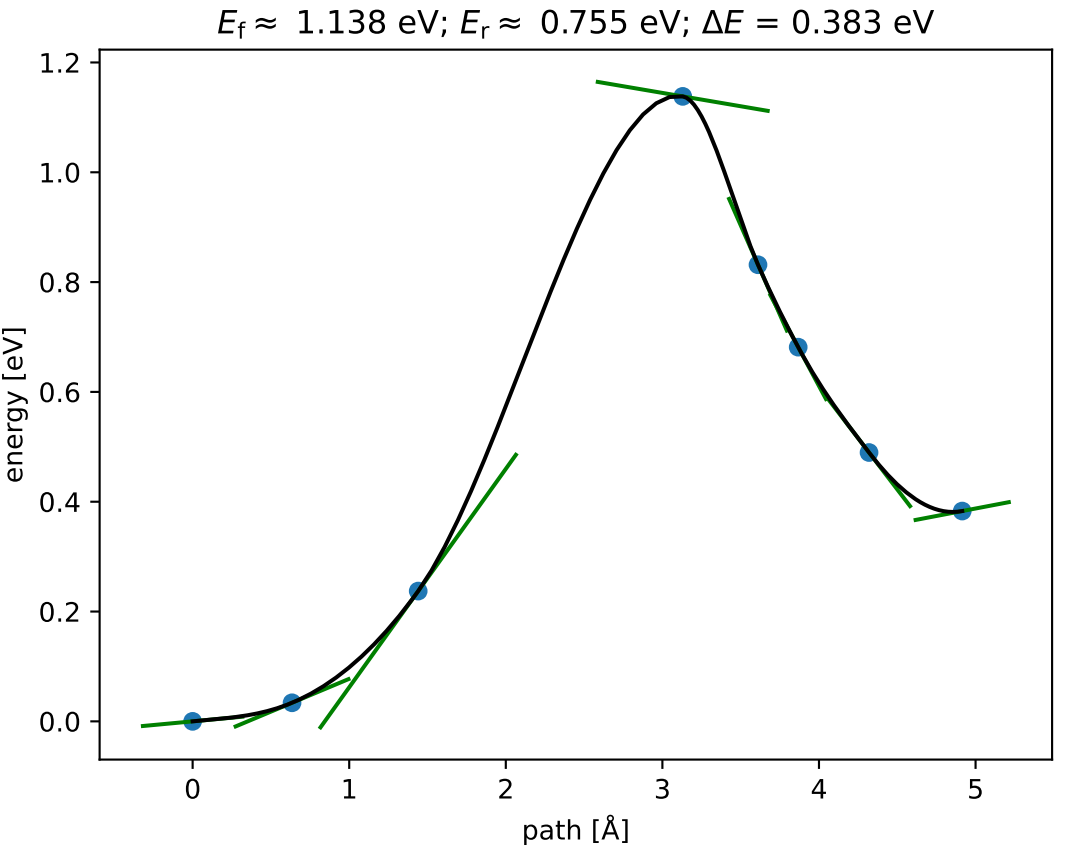
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.138 eV; $E_r \approx$ 0.755 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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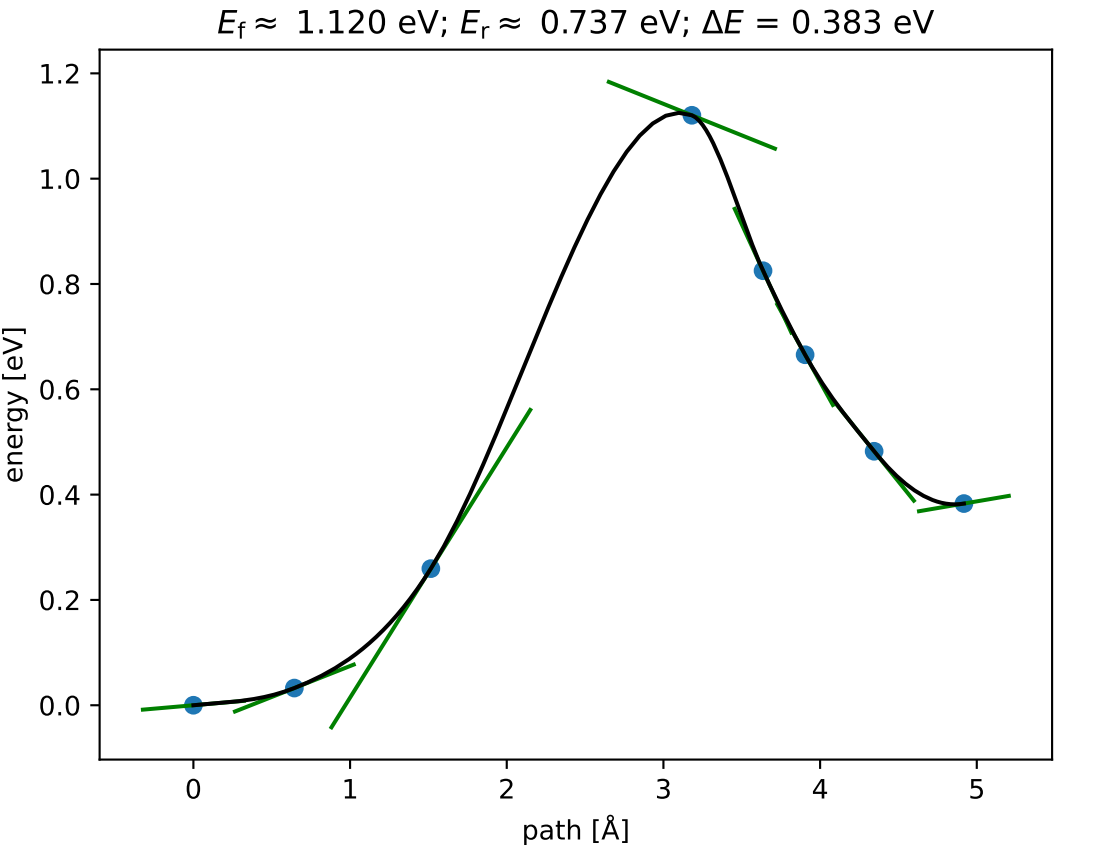
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.120 eV; $E_r \approx$ 0.737 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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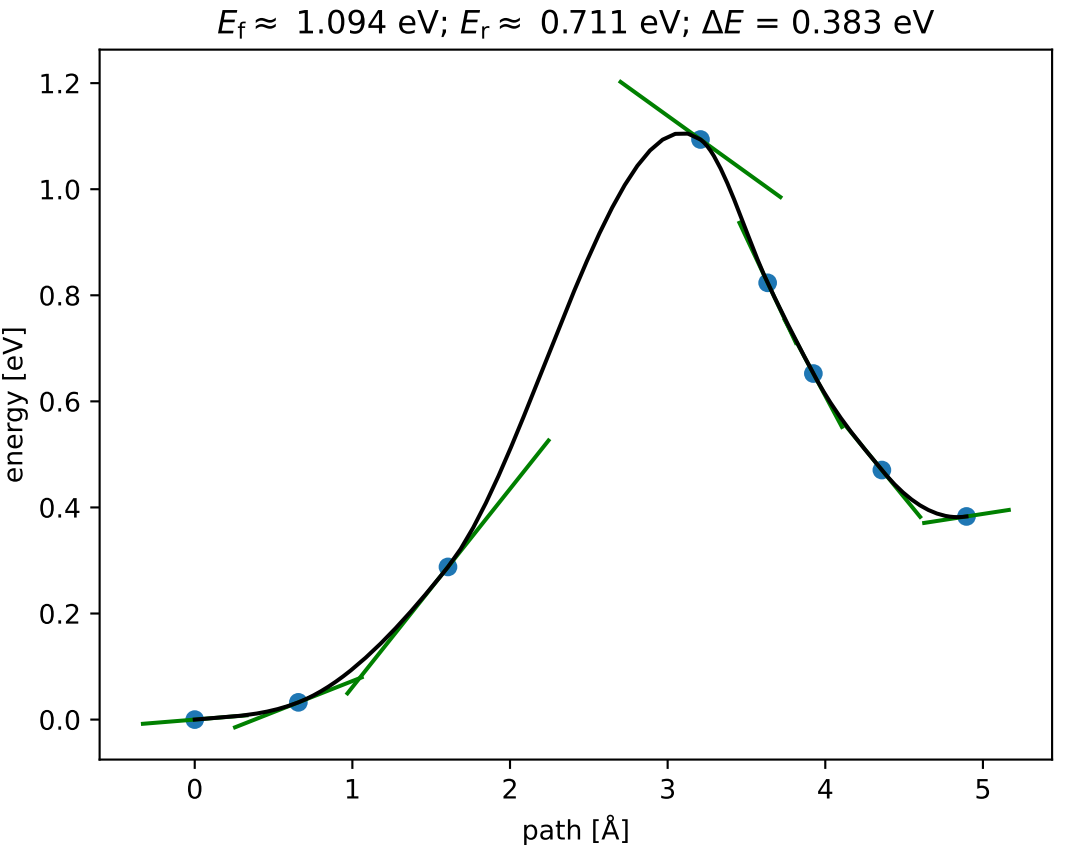
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.094 eV; $E_r \approx$ 0.711 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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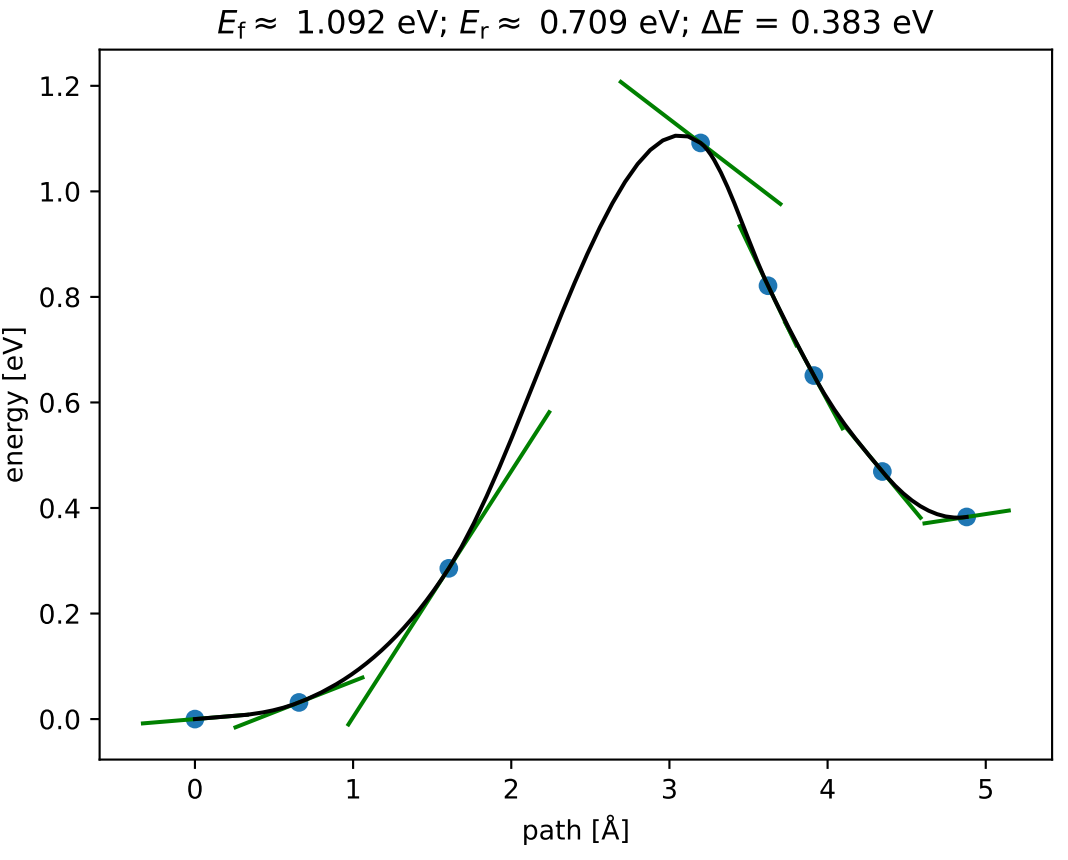
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.092 eV; $E_r \approx$ 0.709 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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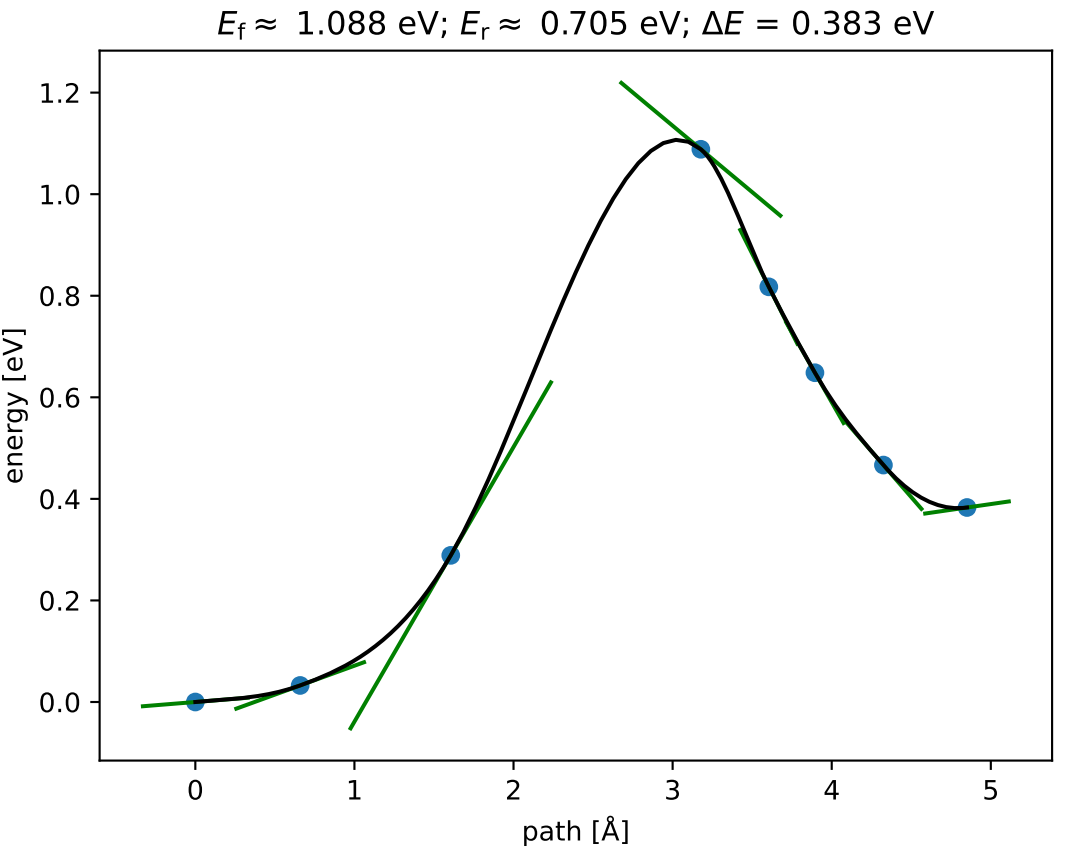
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.088 eV; $E_r \approx$ 0.705 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.4
0.6
0.8
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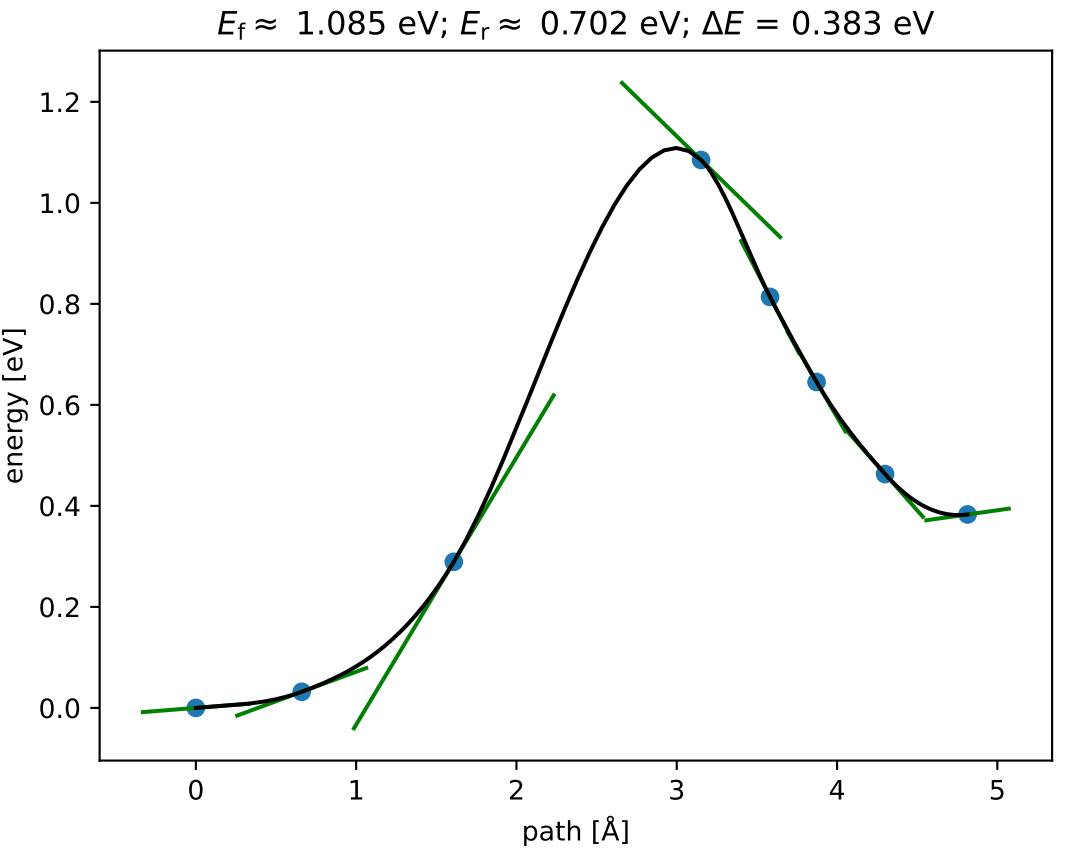
1.2
0
1
2
3
4
5


$E_f \approx$ 1.085 eV; $E_r \approx$ 0.702 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.4
0.6
0.8
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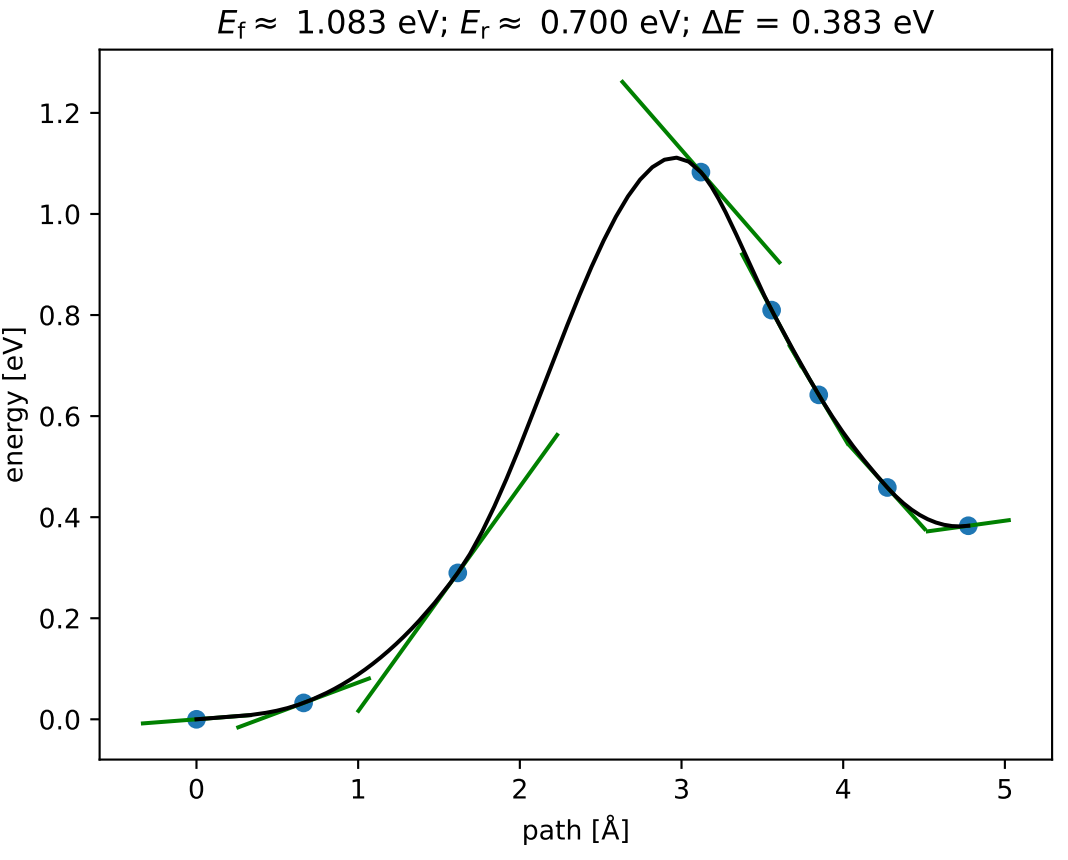
1.2
0
1
2
3
4
5


$E_f \approx$ 1.083 eV; $E_r \approx$ 0.700 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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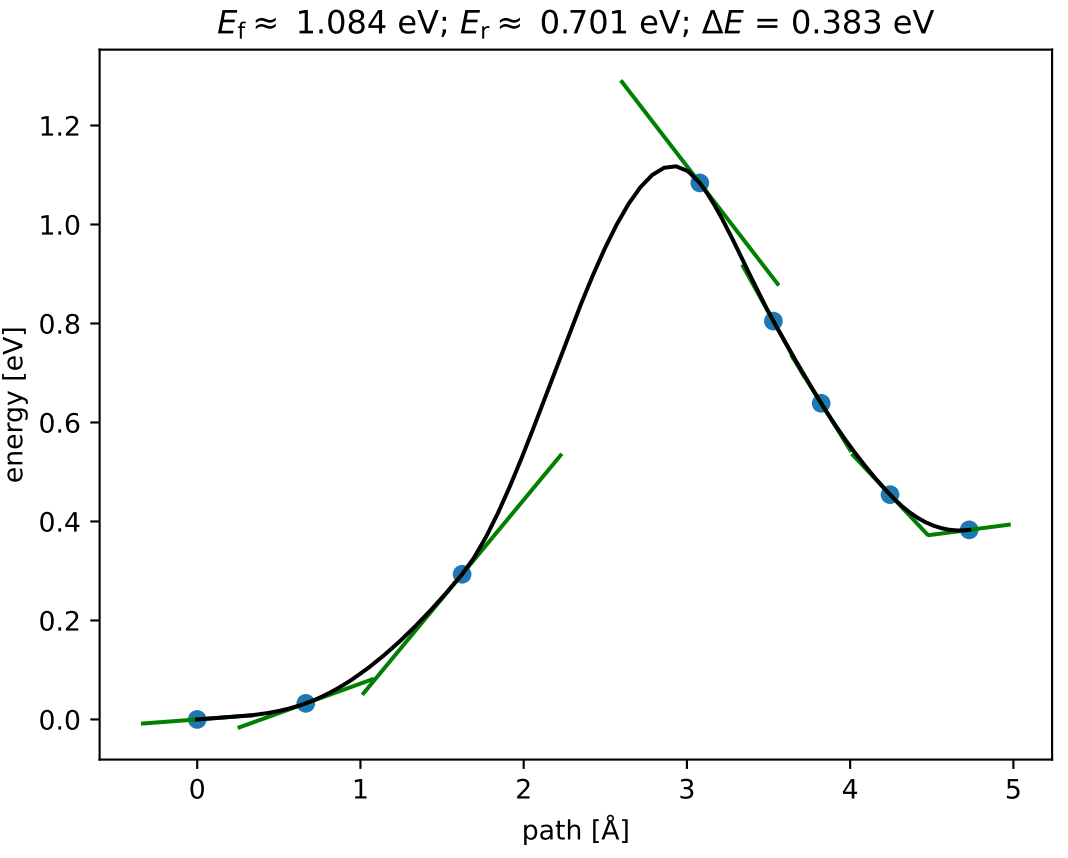
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.084 eV; $E_r \approx$ 0.701 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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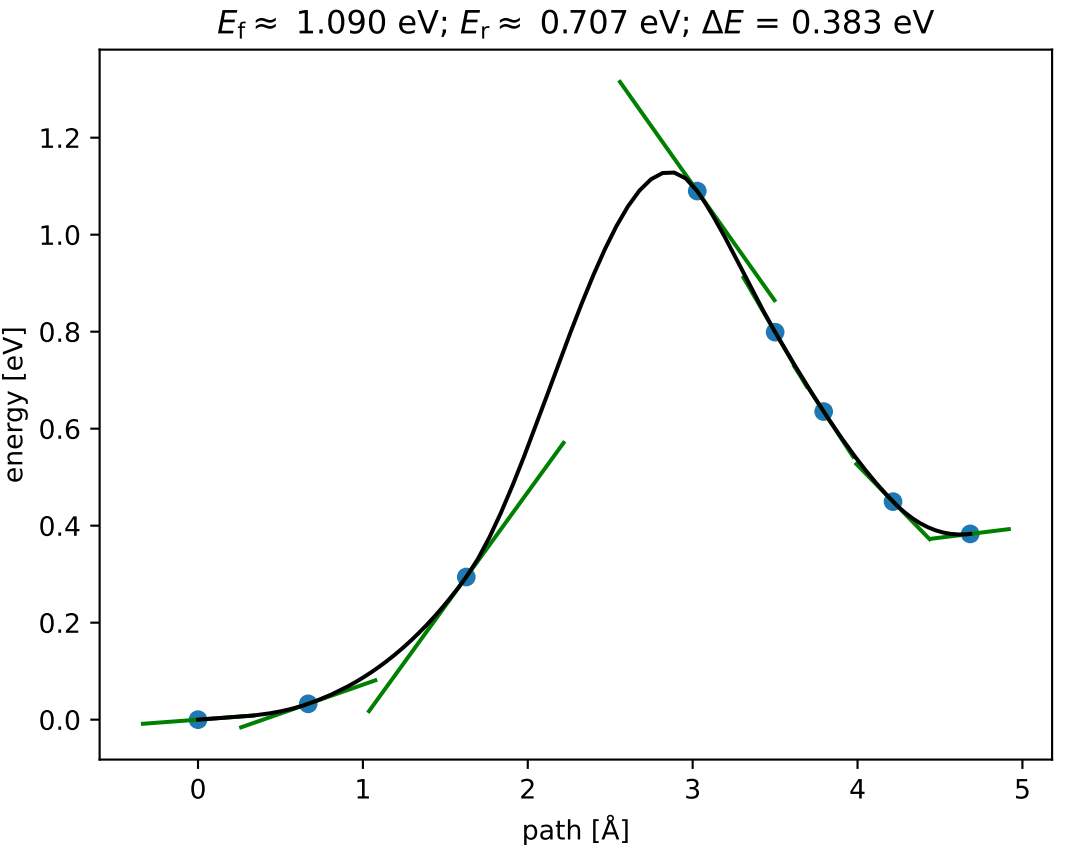
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.090 eV; $E_r \approx$ 0.707 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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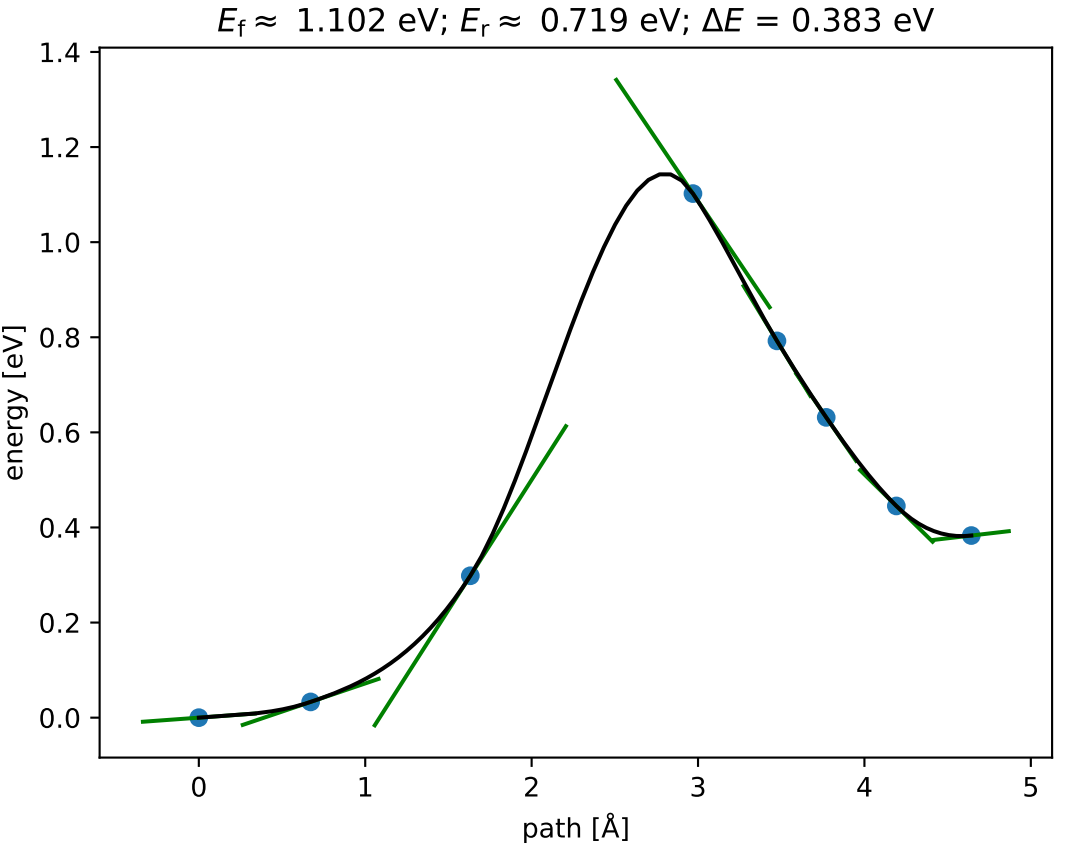
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.102 eV; $E_r \approx$ 0.719 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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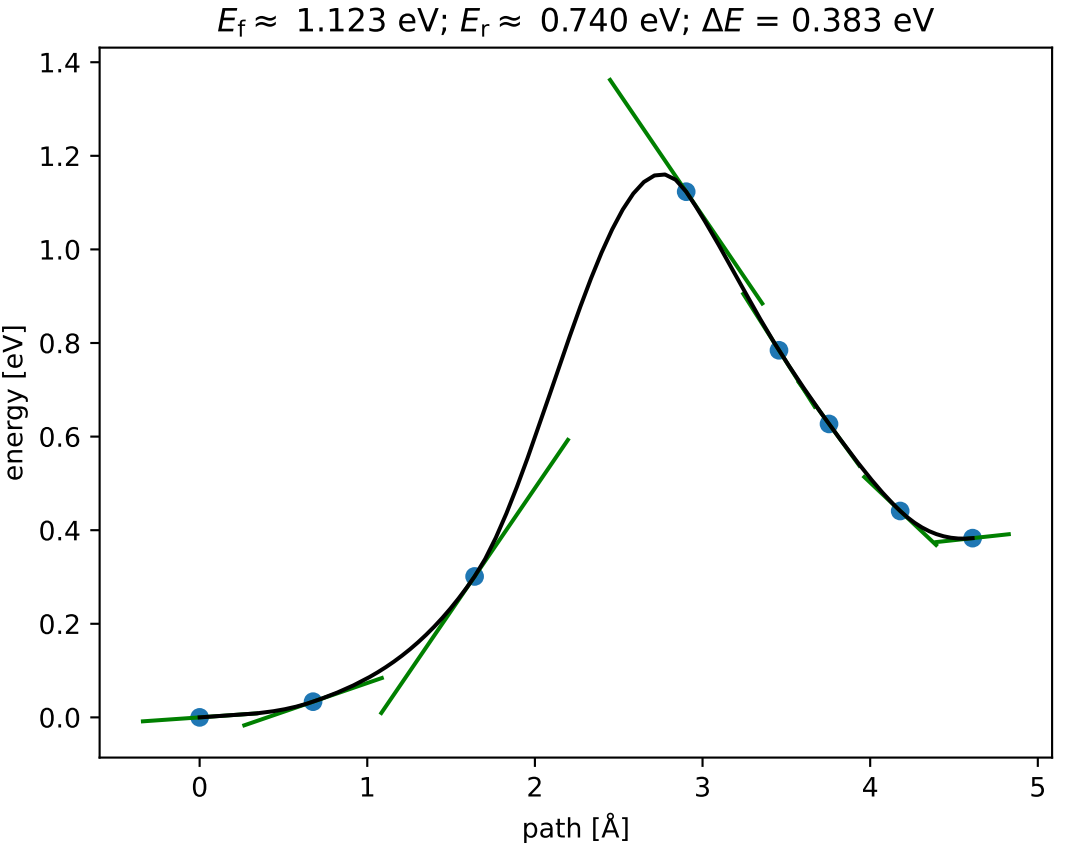
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.123 eV; $E_r \approx$ 0.740 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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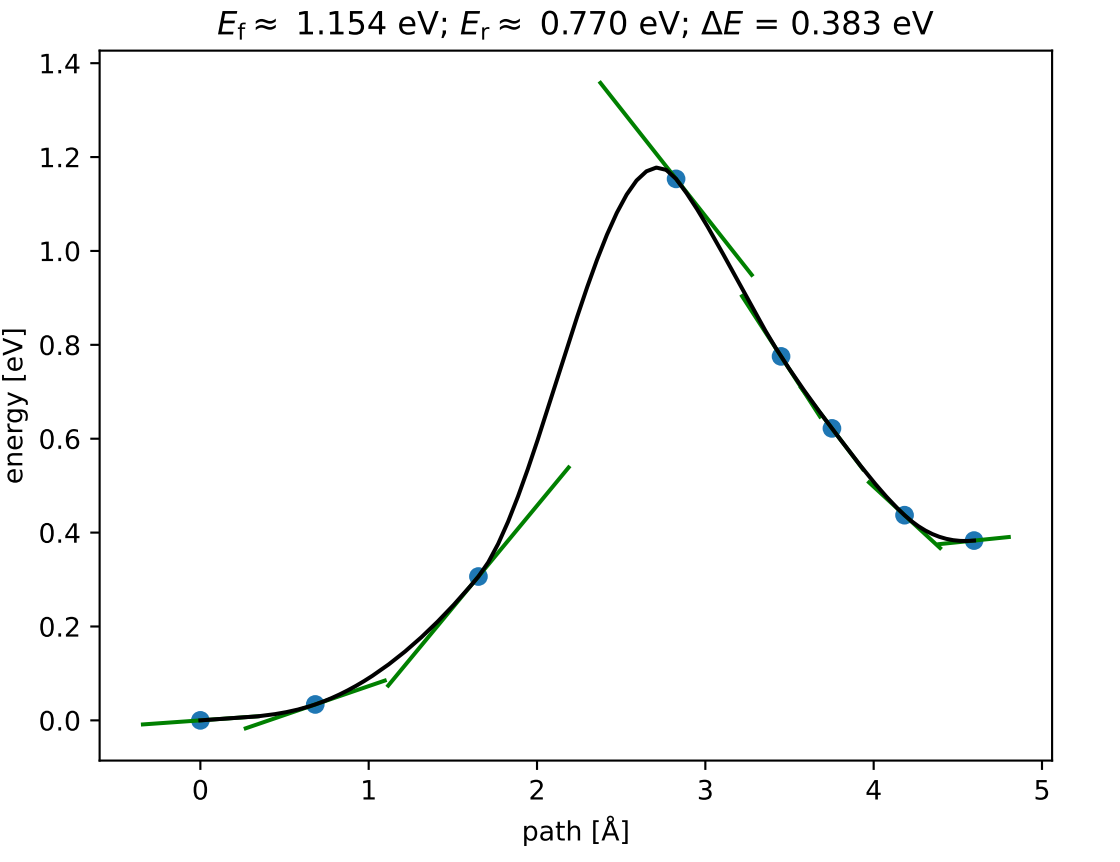
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.154 eV; $E_r \approx$ 0.770 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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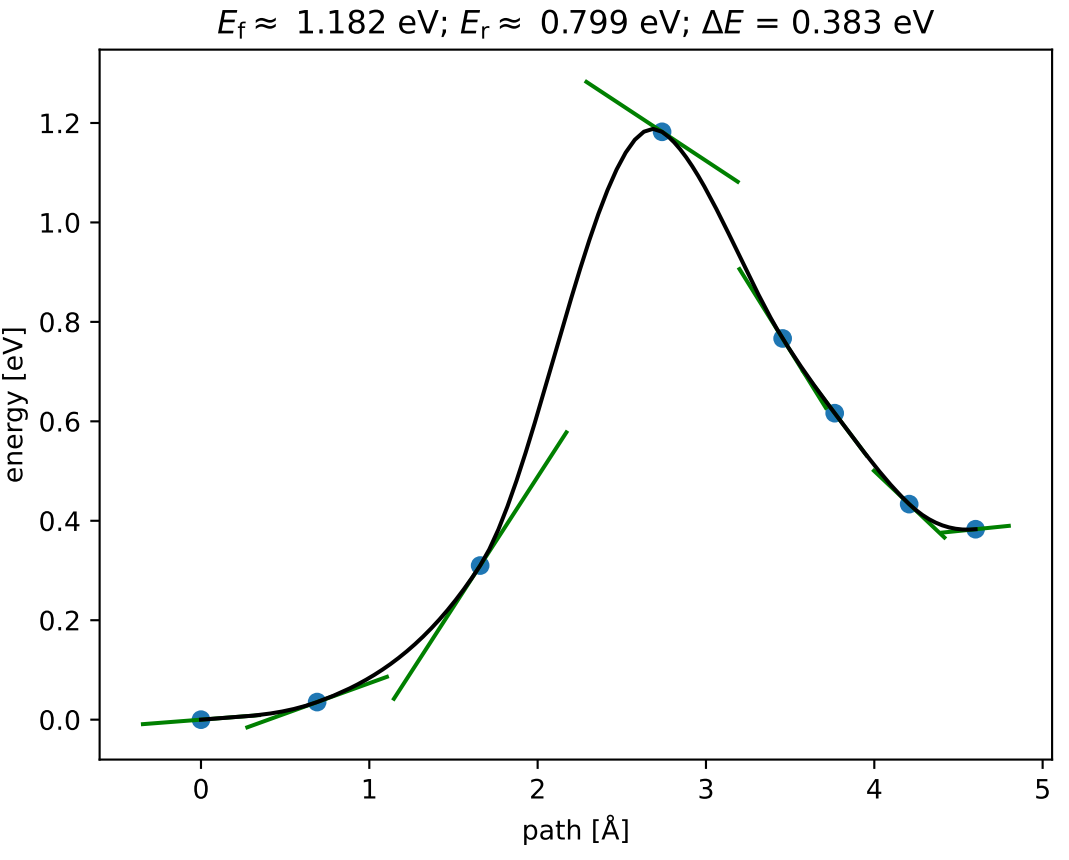
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5


$E_f \approx$ 1.182 eV; $E_r \approx$ 0.799 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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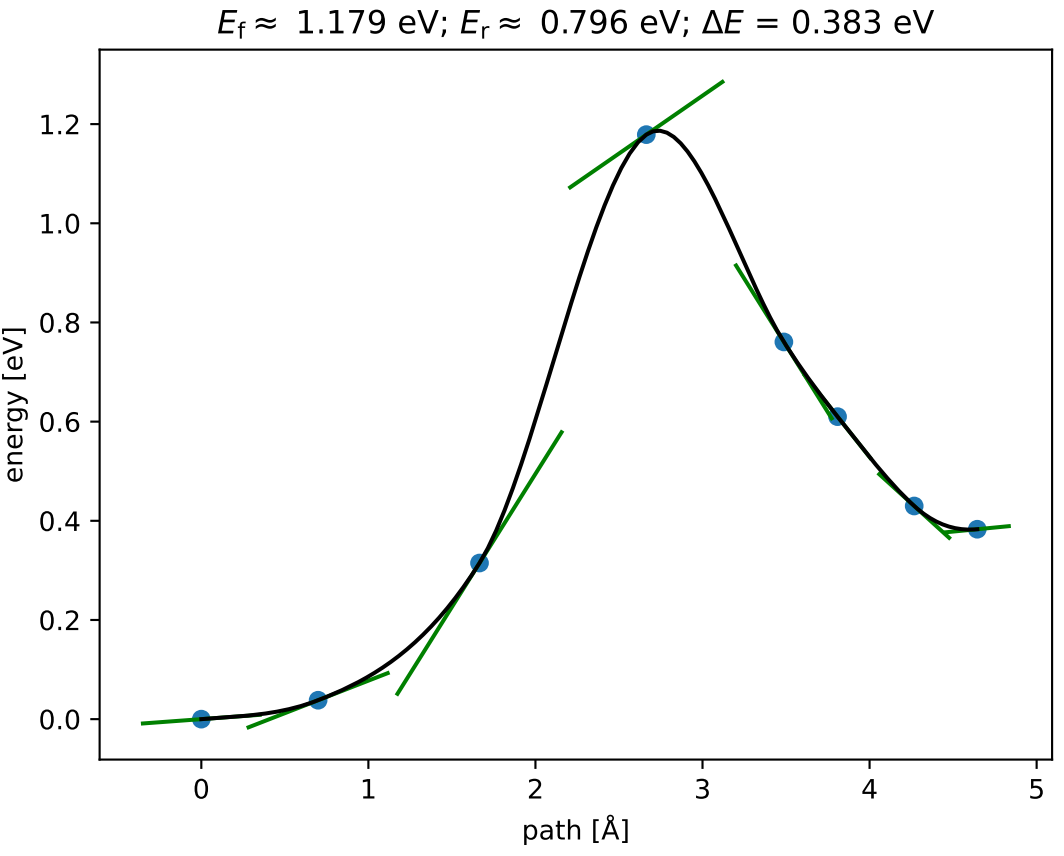
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.179 eV; $E_r \approx$ 0.796 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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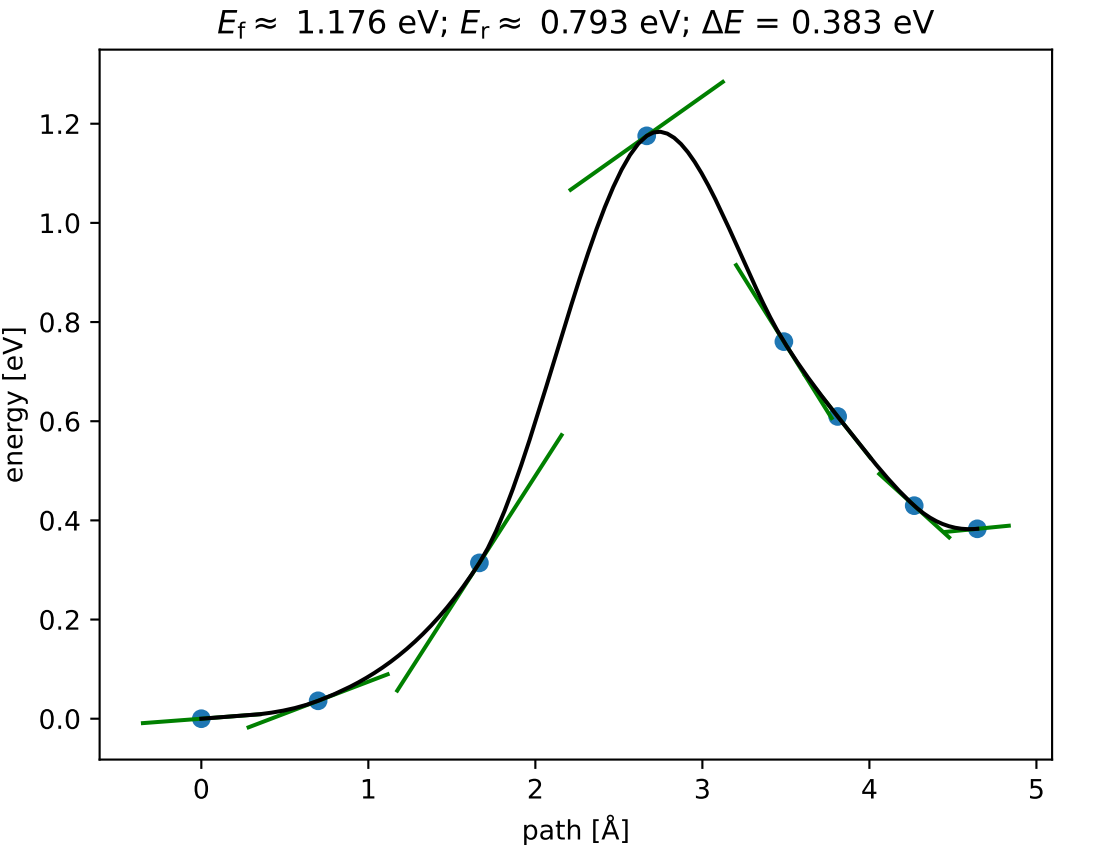
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.176 eV; $E_r \approx$ 0.793 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.2
0.4
0.6
0.8
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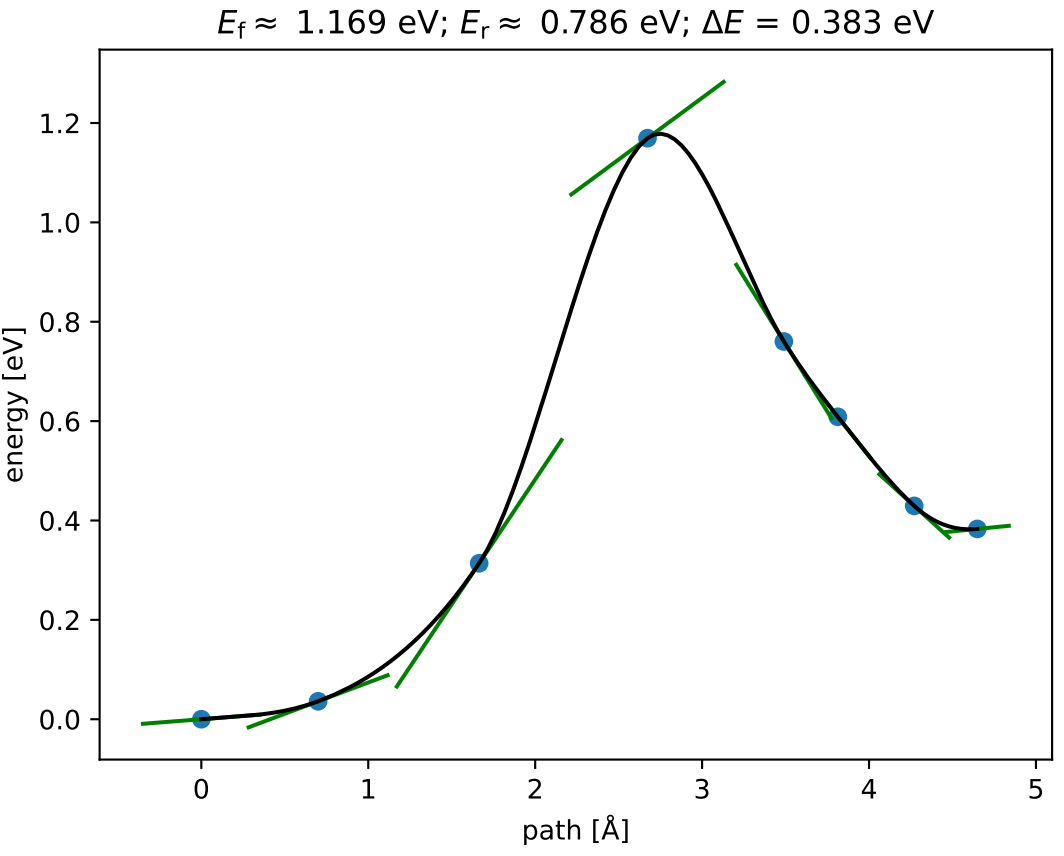
1.2
0
1
2
3
4
5


$E_f \approx$ 1.169 eV; $E_r \approx$ 0.786 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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0.2
0.4
0.6
0.8
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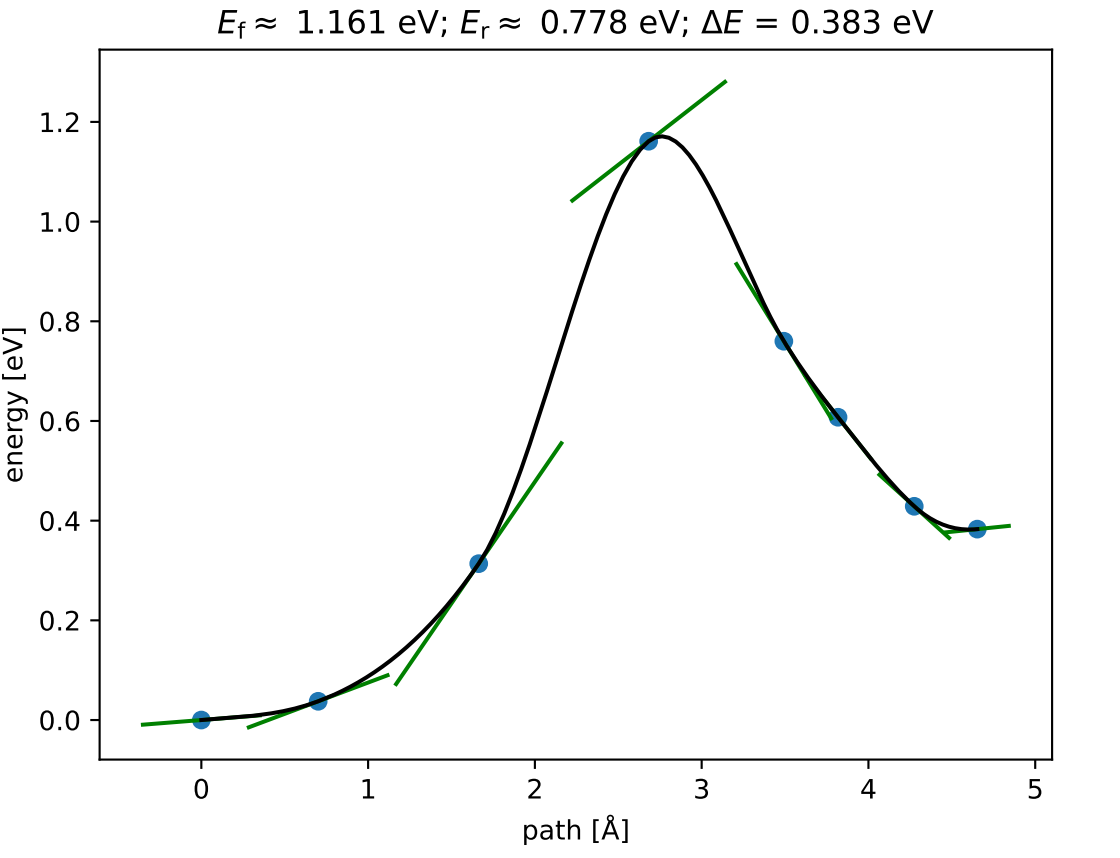
1.2
0
1
2
3
4
5


$E_f \approx$ 1.161 eV; $E_r \approx$ 0.778 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
0.0
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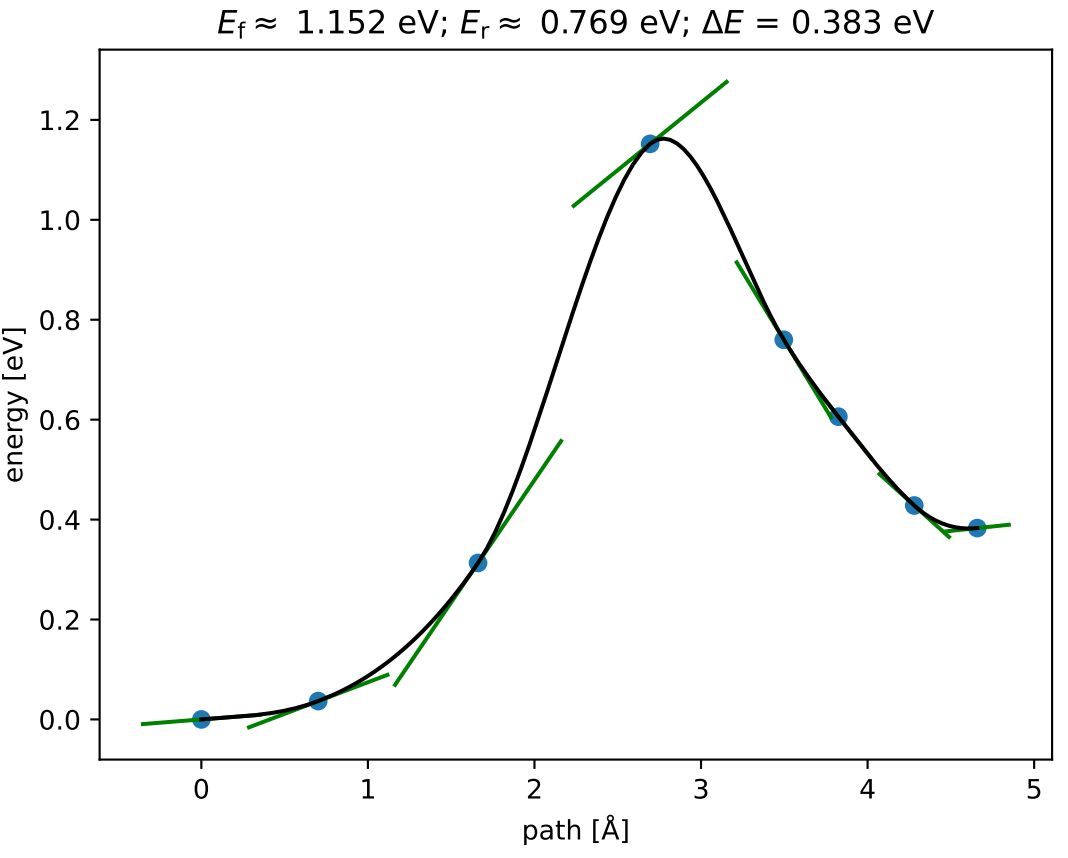
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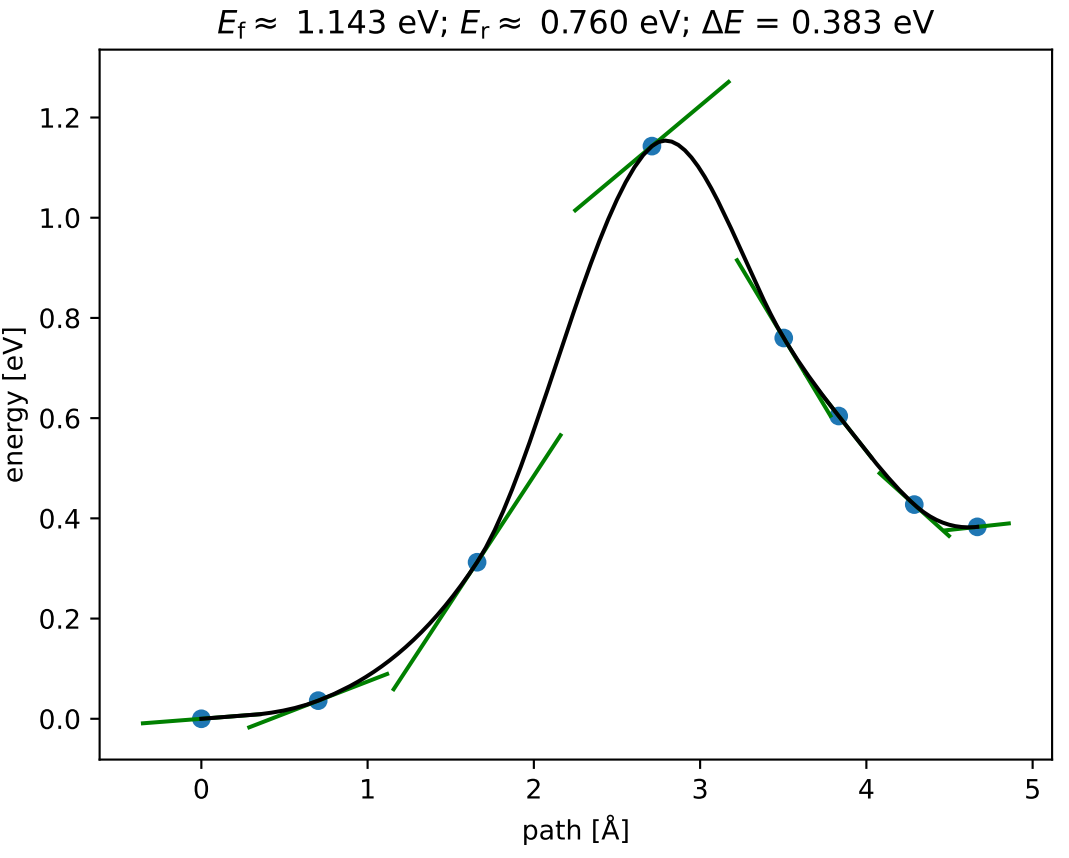
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path [Å]
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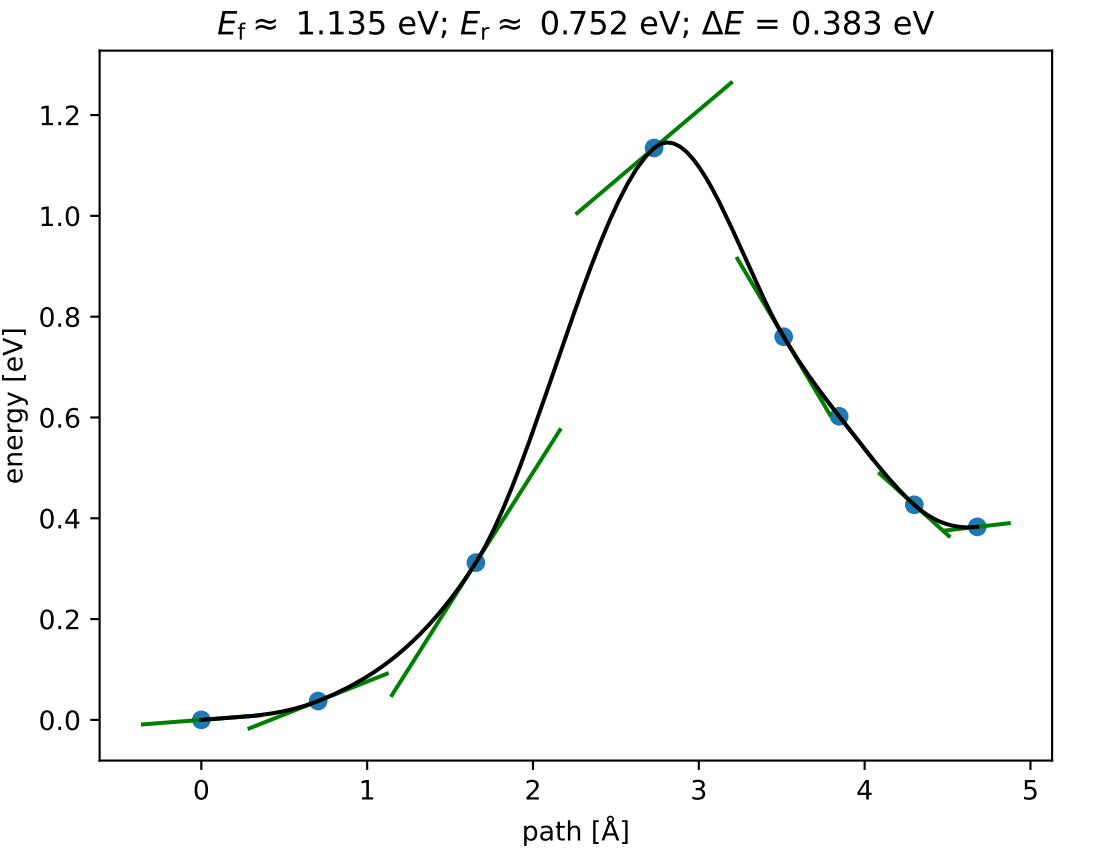
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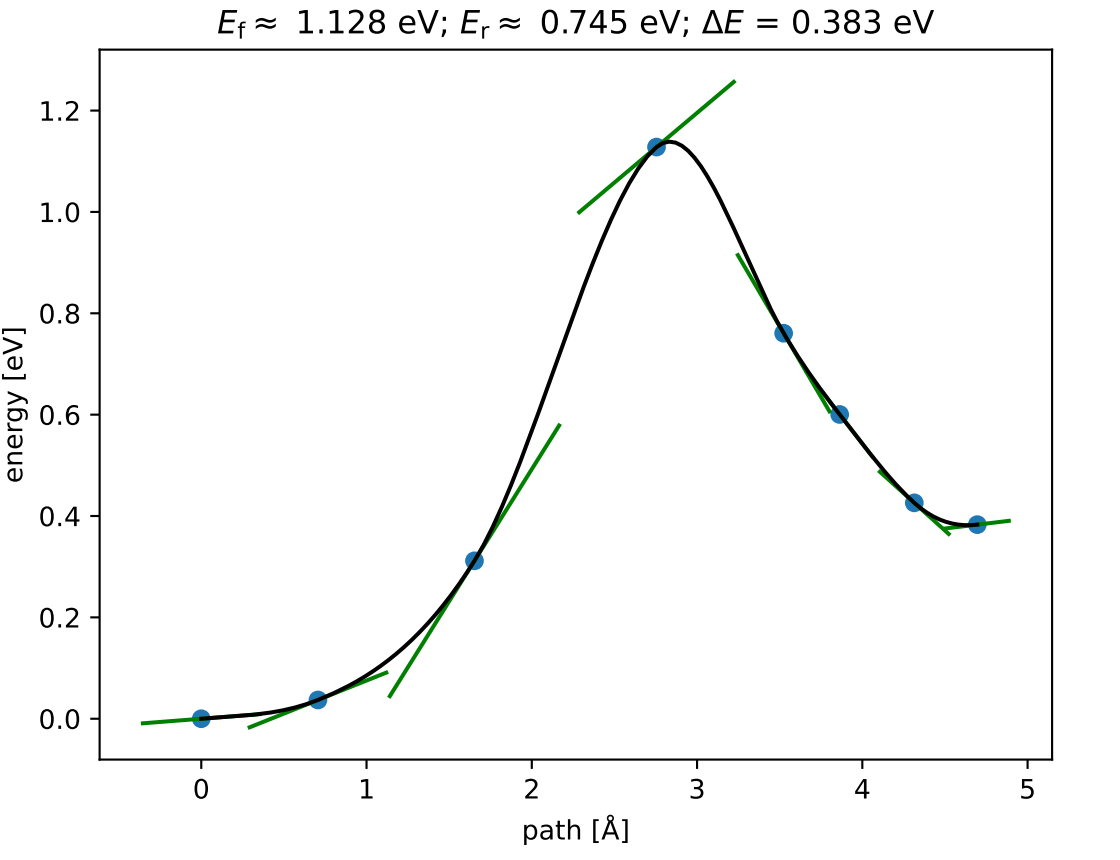
$E_f \approx$ 1.128 eV; $E_r \approx$ 0.745 eV; ΔE = 0.383 eV
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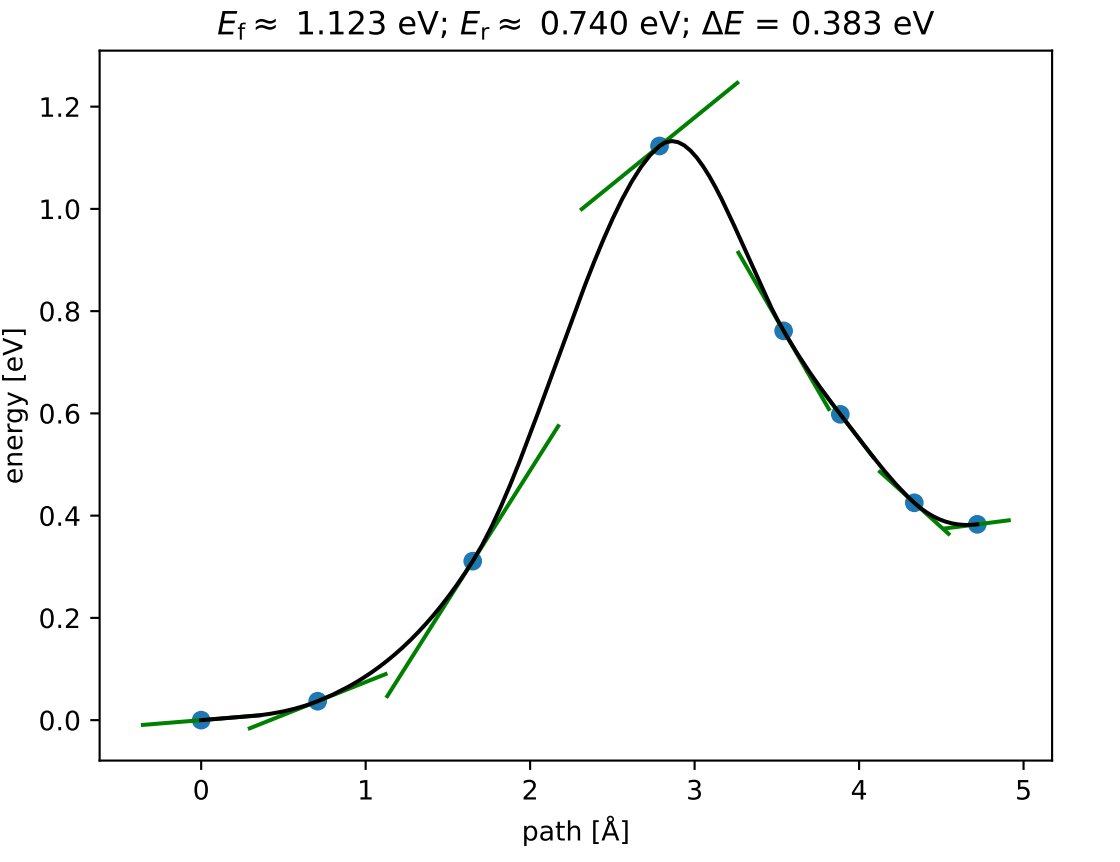
$E_f \approx$ 1.123 eV; $E_r \approx$ 0.740 eV; ΔE = 0.383 eV
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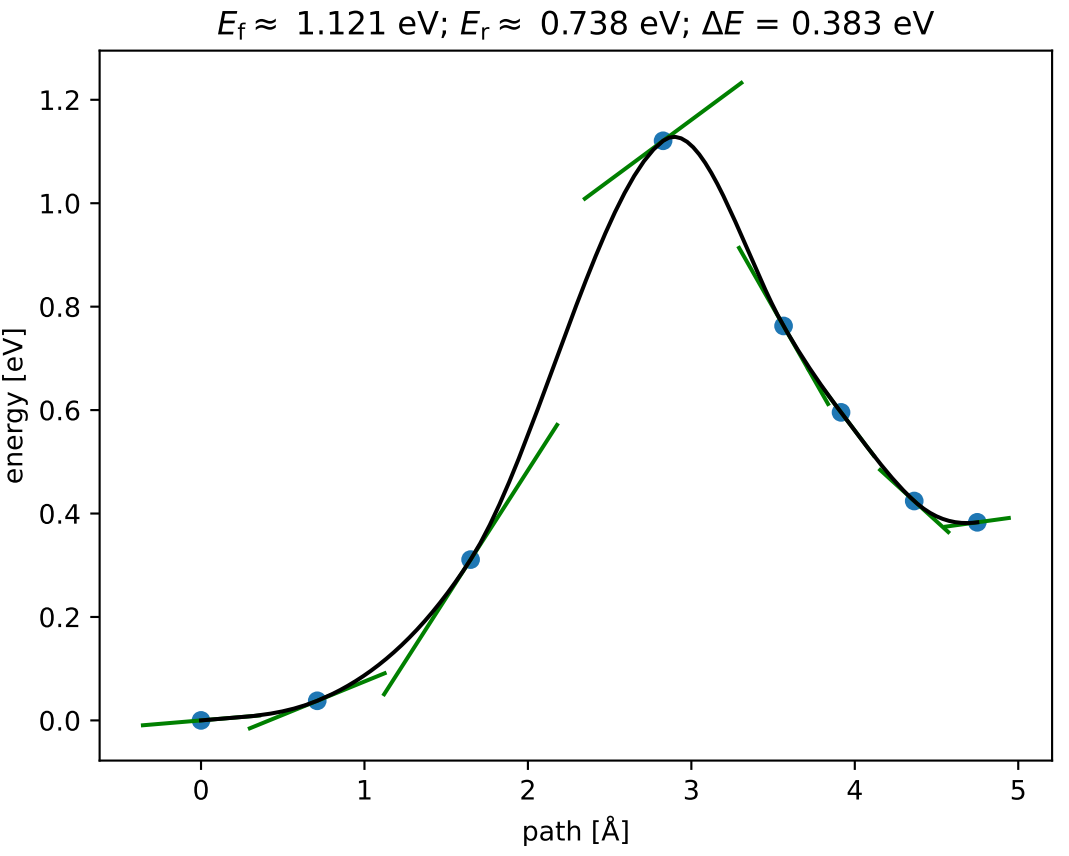
$E_f \approx$ 1.121 eV; $E_r \approx$ 0.738 eV; ΔE = 0.383 eV
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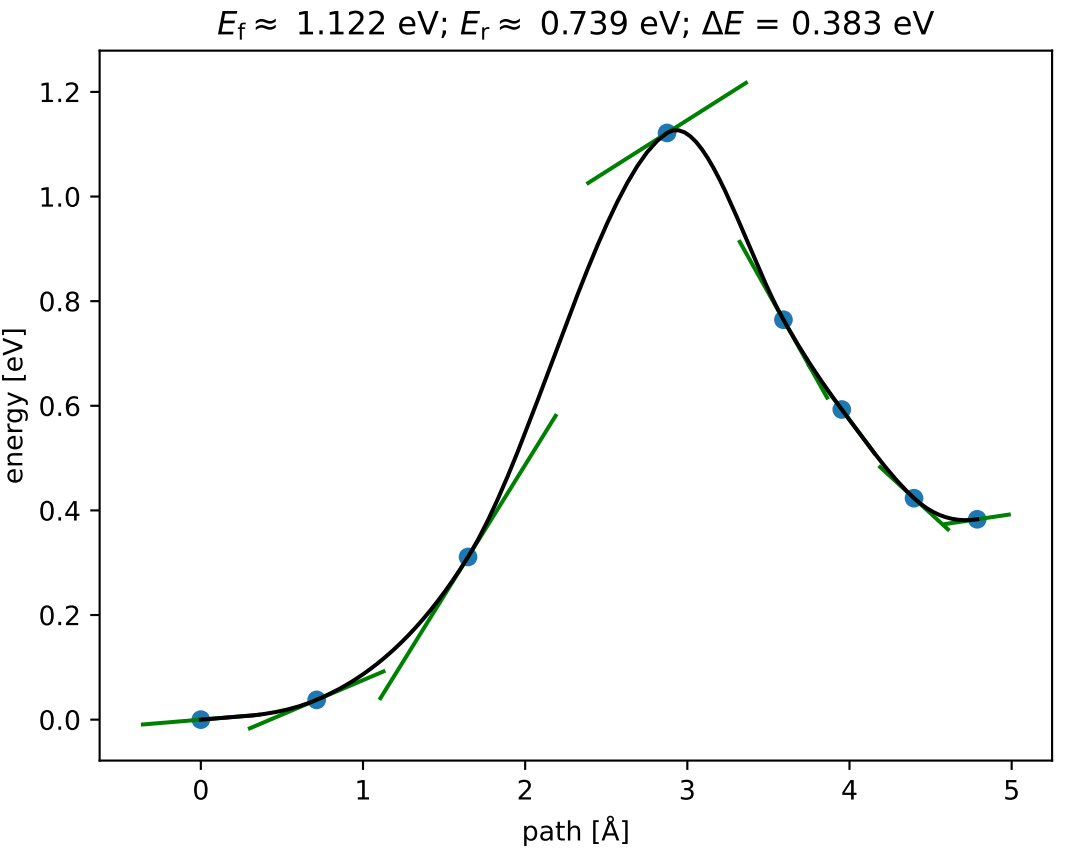
$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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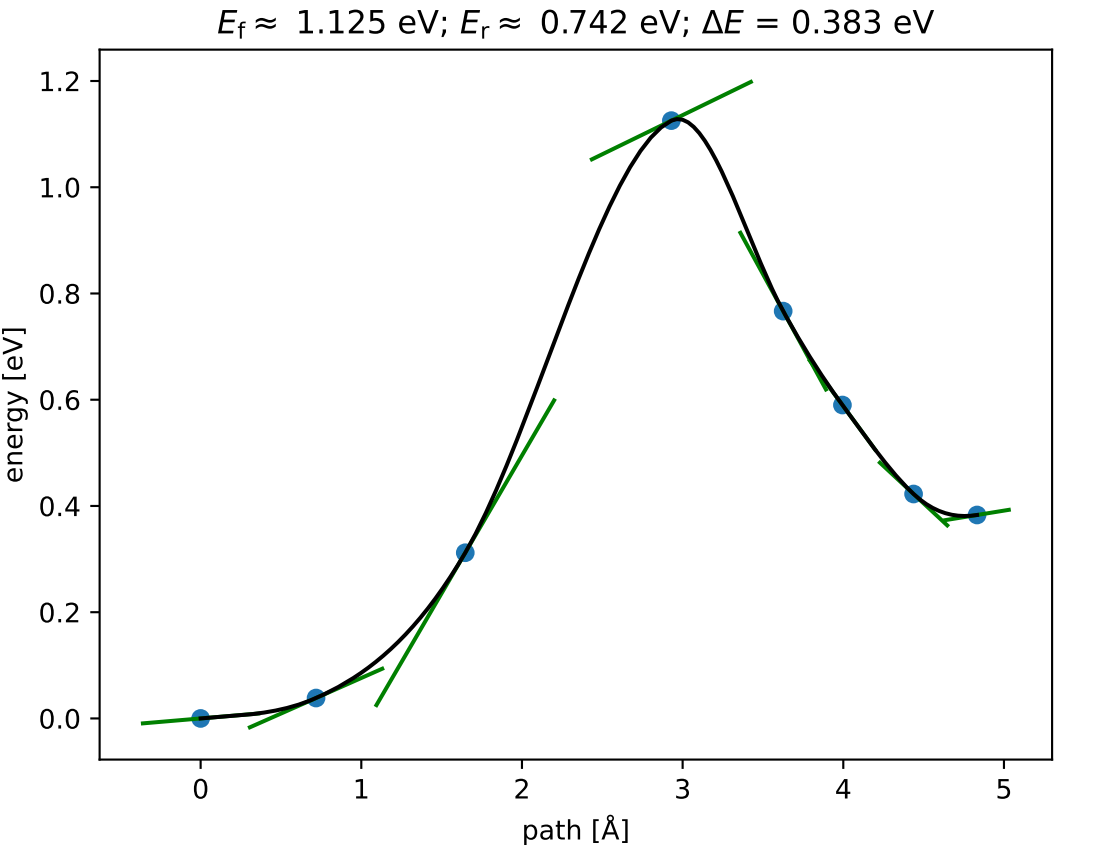
$E_f \approx$ 1.125 eV; $E_r \approx$ 0.742 eV; ΔE = 0.383 eV
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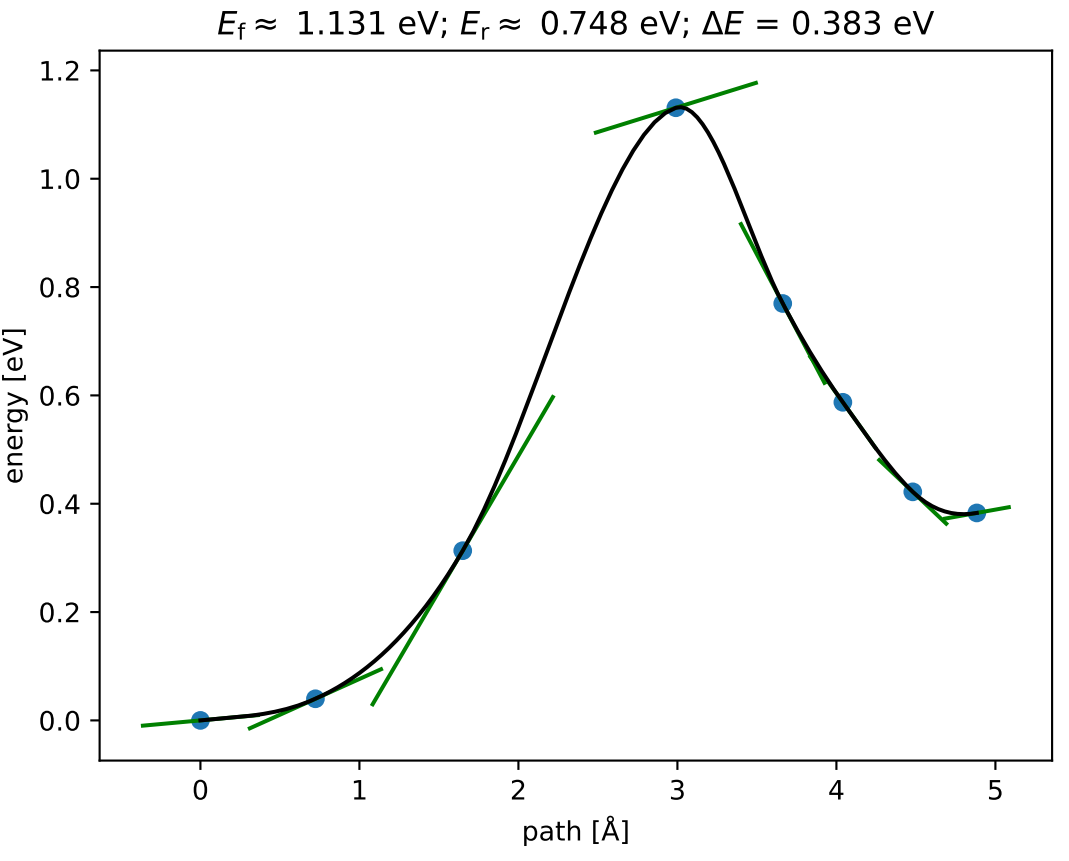
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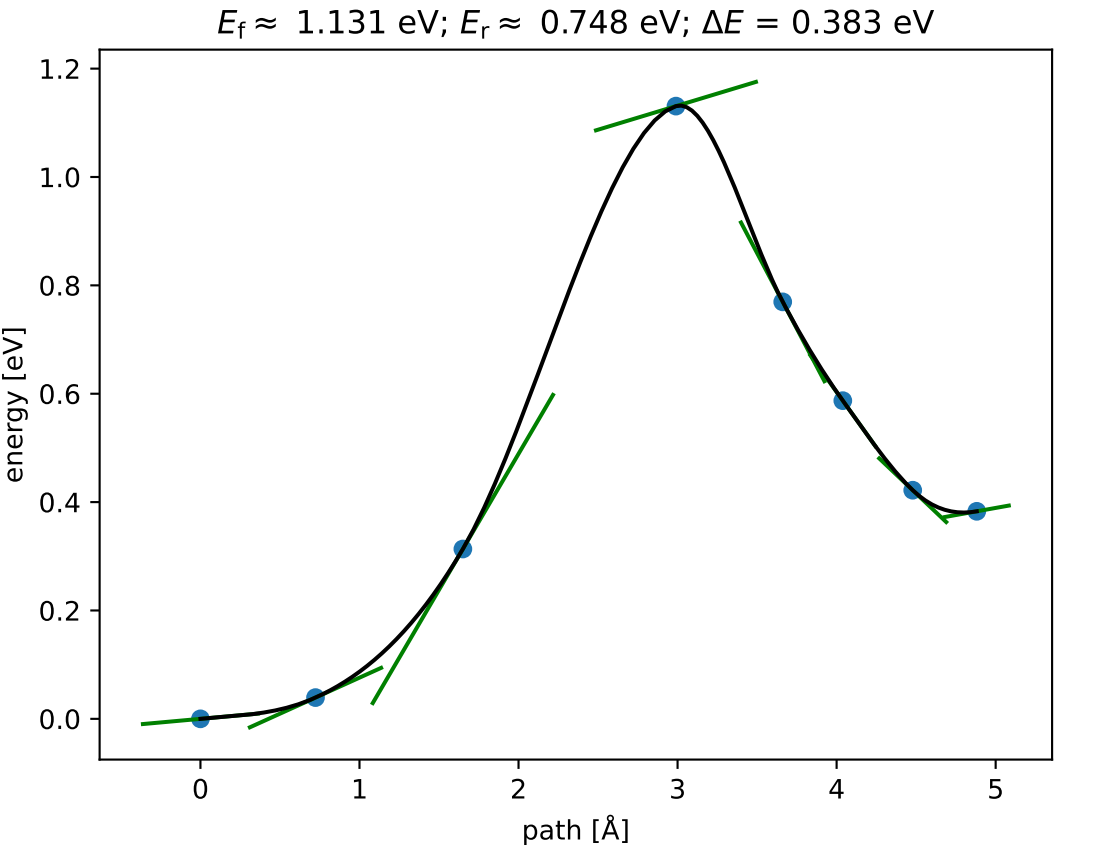
$E_f \approx$ 1.131 eV; $E_r \approx$ 0.748 eV; ΔE = 0.383 eV
energy [eV]
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0.8
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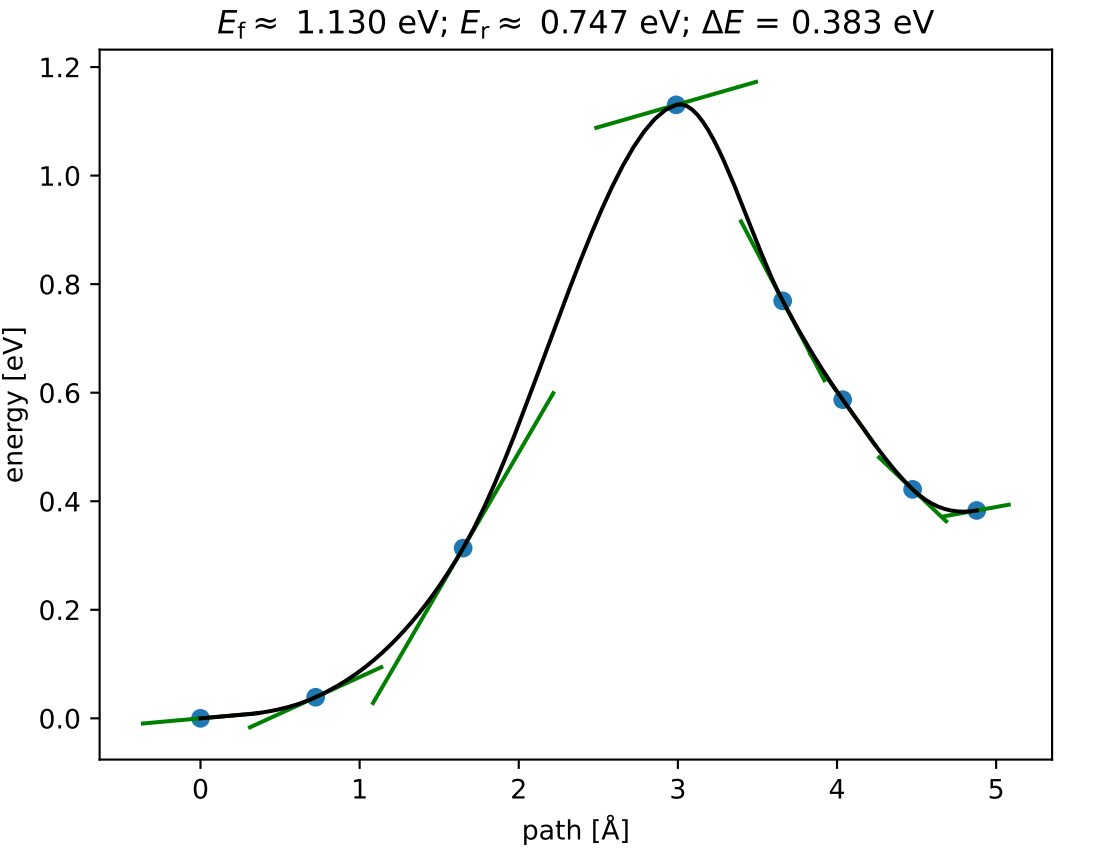
$E_f \approx$ 1.130 eV; $E_r \approx$ 0.747 eV; ΔE = 0.383 eV
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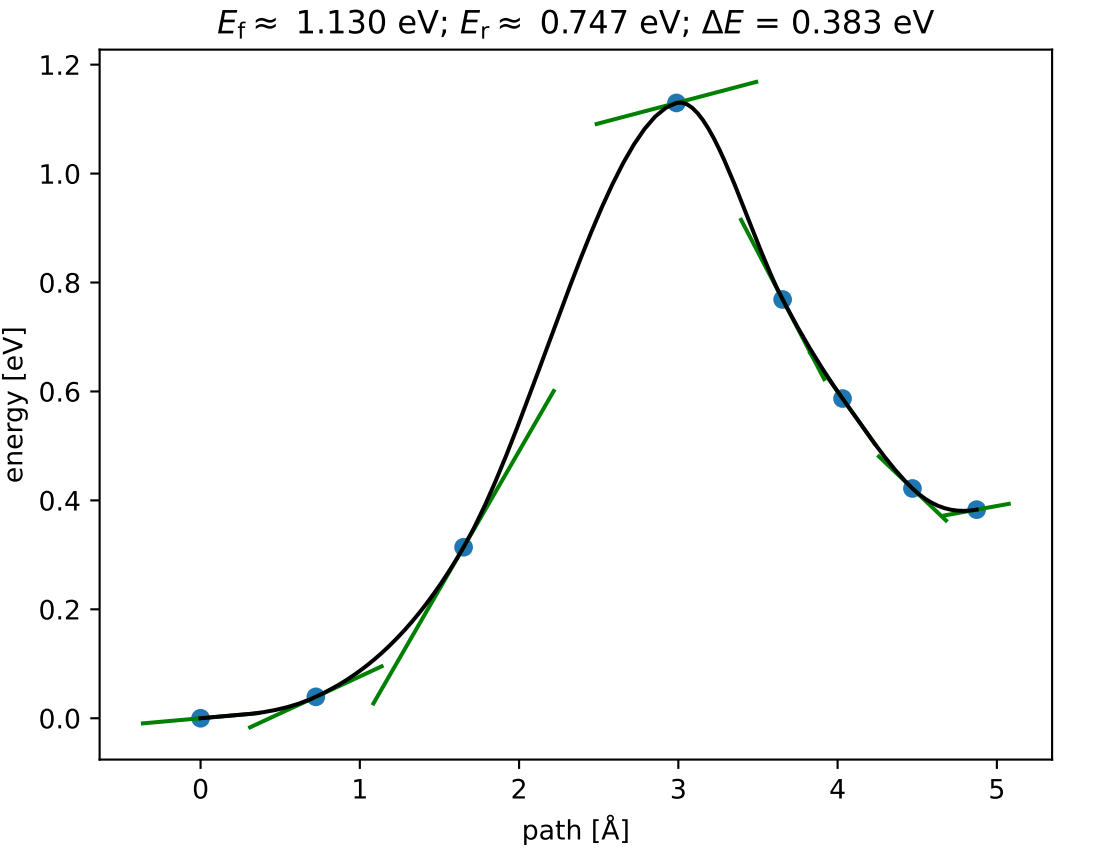
$E_f \approx$ 1.130 eV; $E_r \approx$ 0.747 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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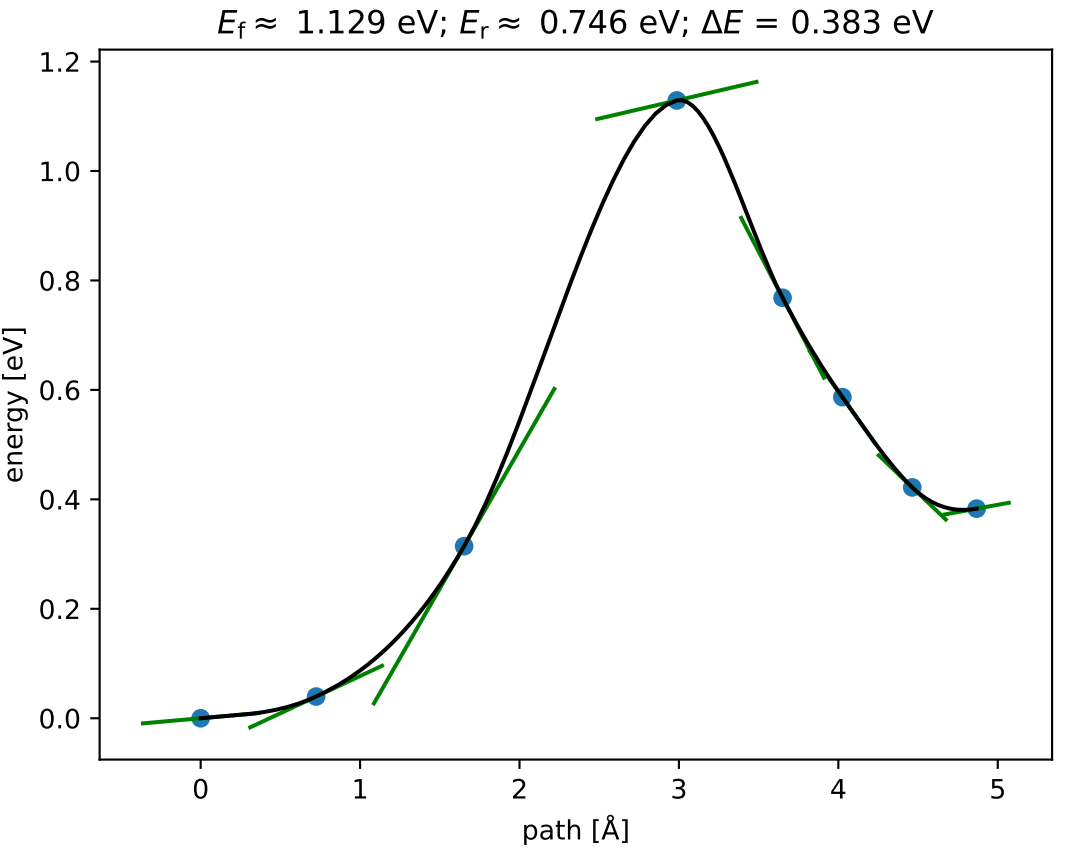
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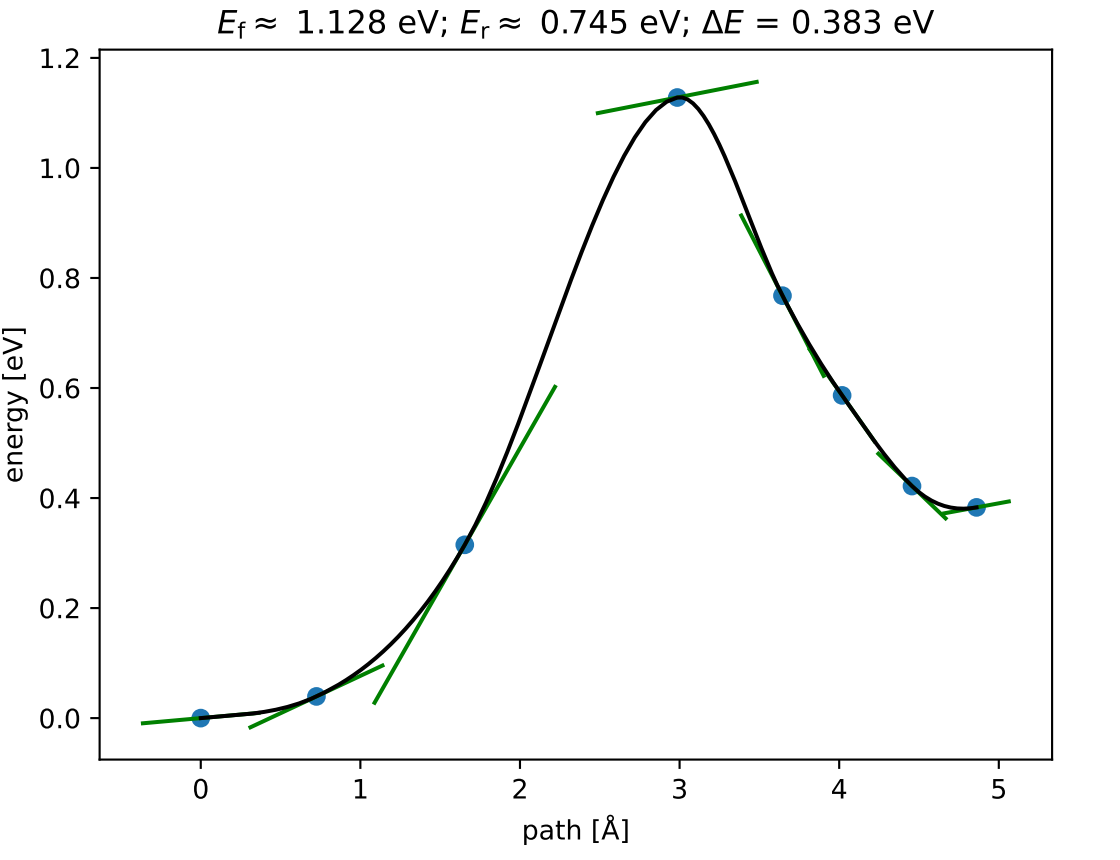
$E_f \approx$ 1.128 eV; $E_r \approx$ 0.745 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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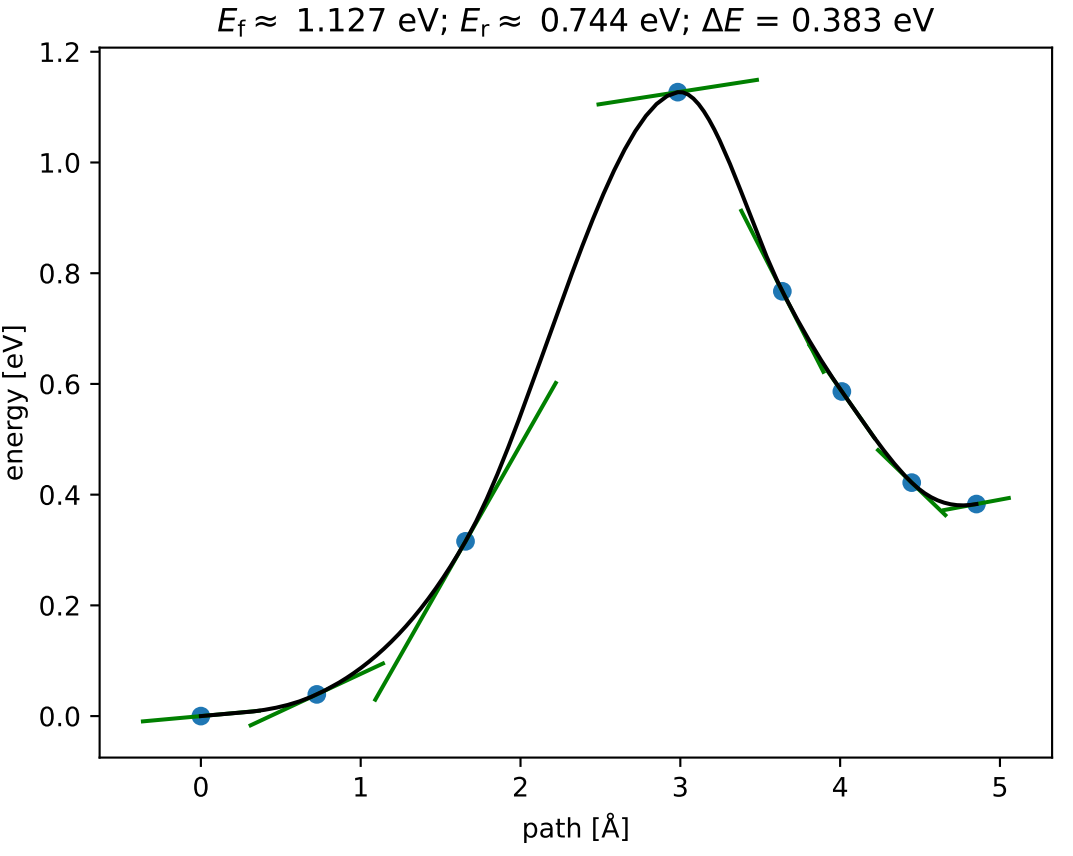
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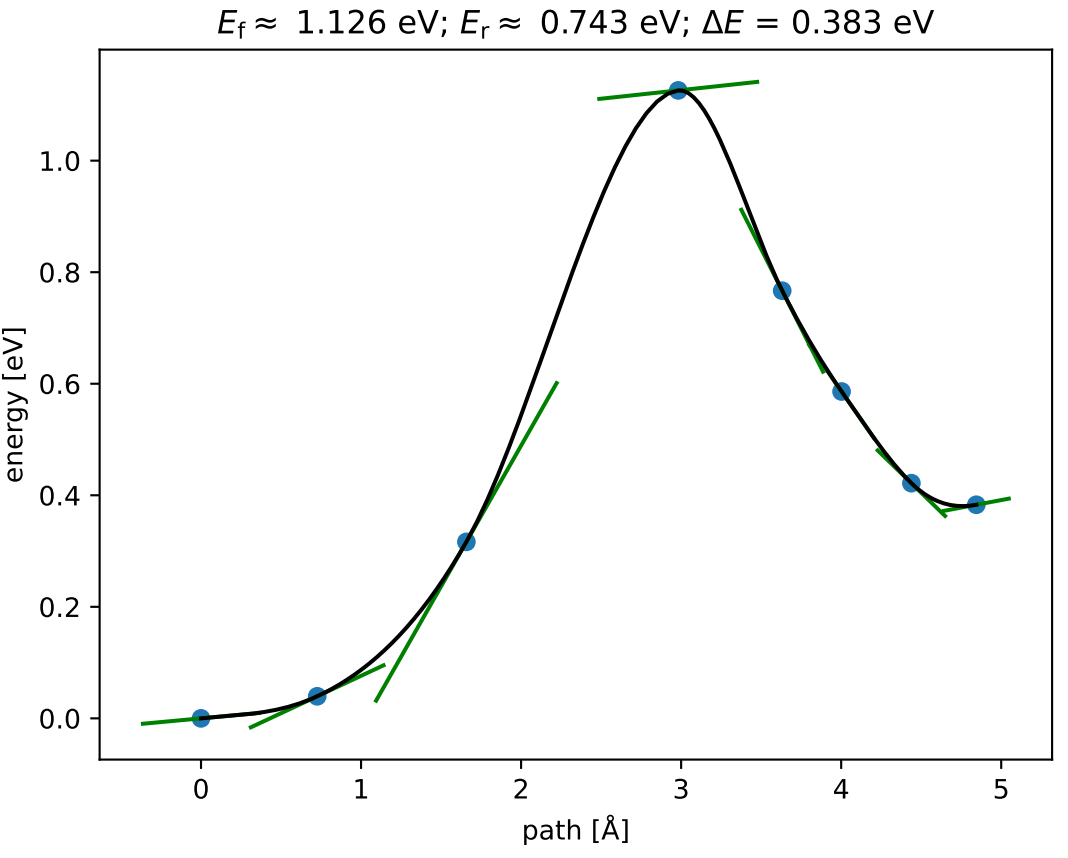
$E_f \approx$ 1.126 eV; $E_r \approx$ 0.743 eV; ΔE = 0.383 eV
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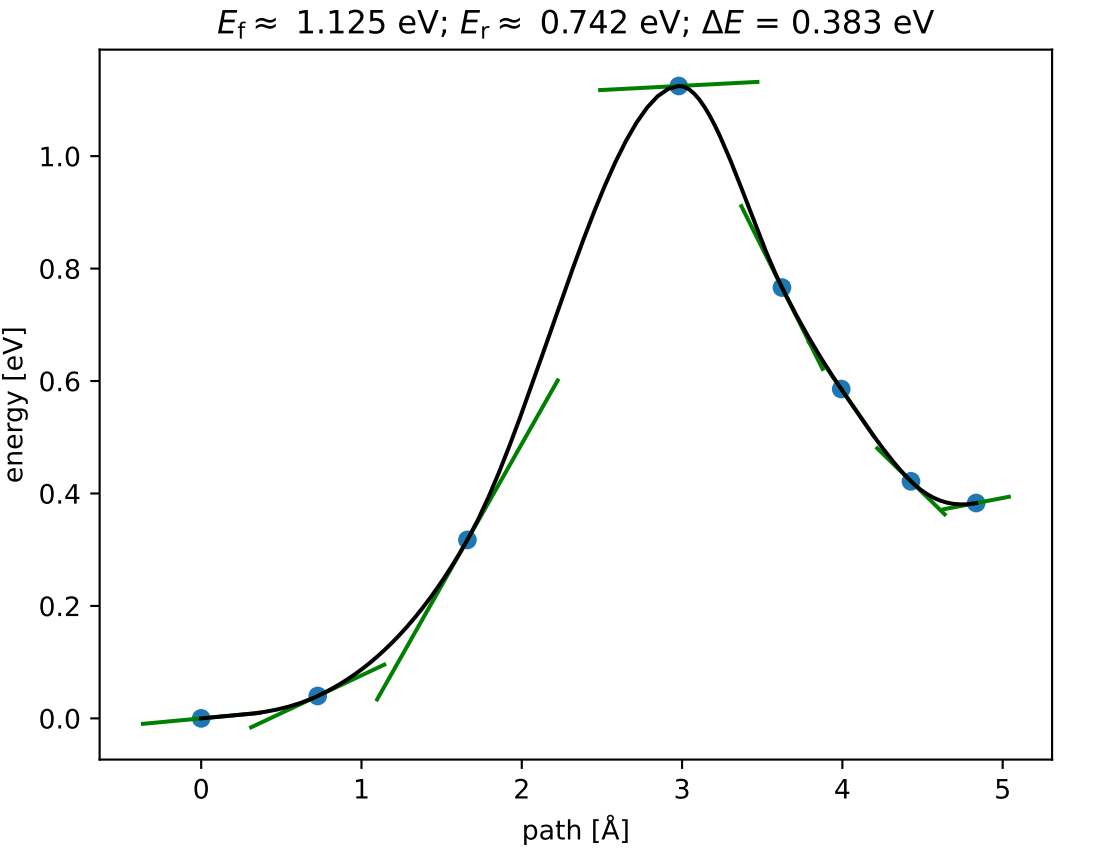
$E_f \approx$ 1.125 eV; $E_r \approx$ 0.742 eV; ΔE = 0.383 eV
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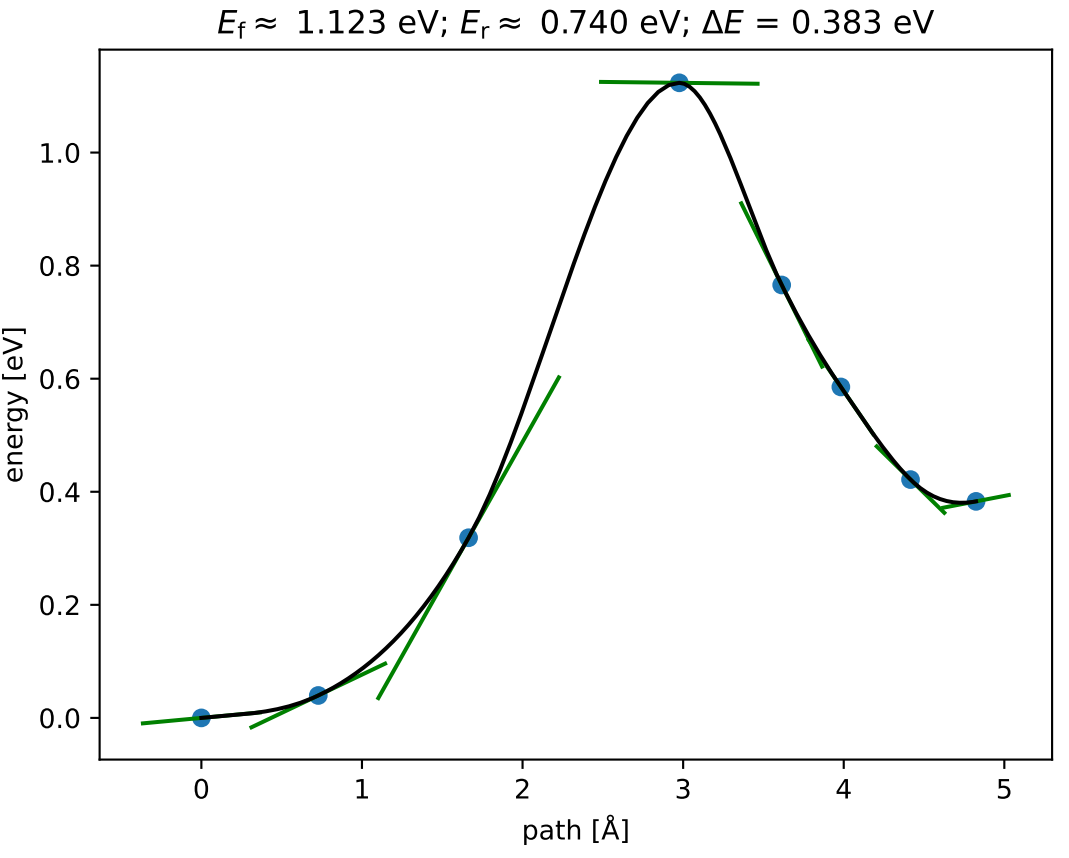
$E_f \approx$ 1.123 eV; $E_r \approx$ 0.740 eV; ΔE = 0.383 eV
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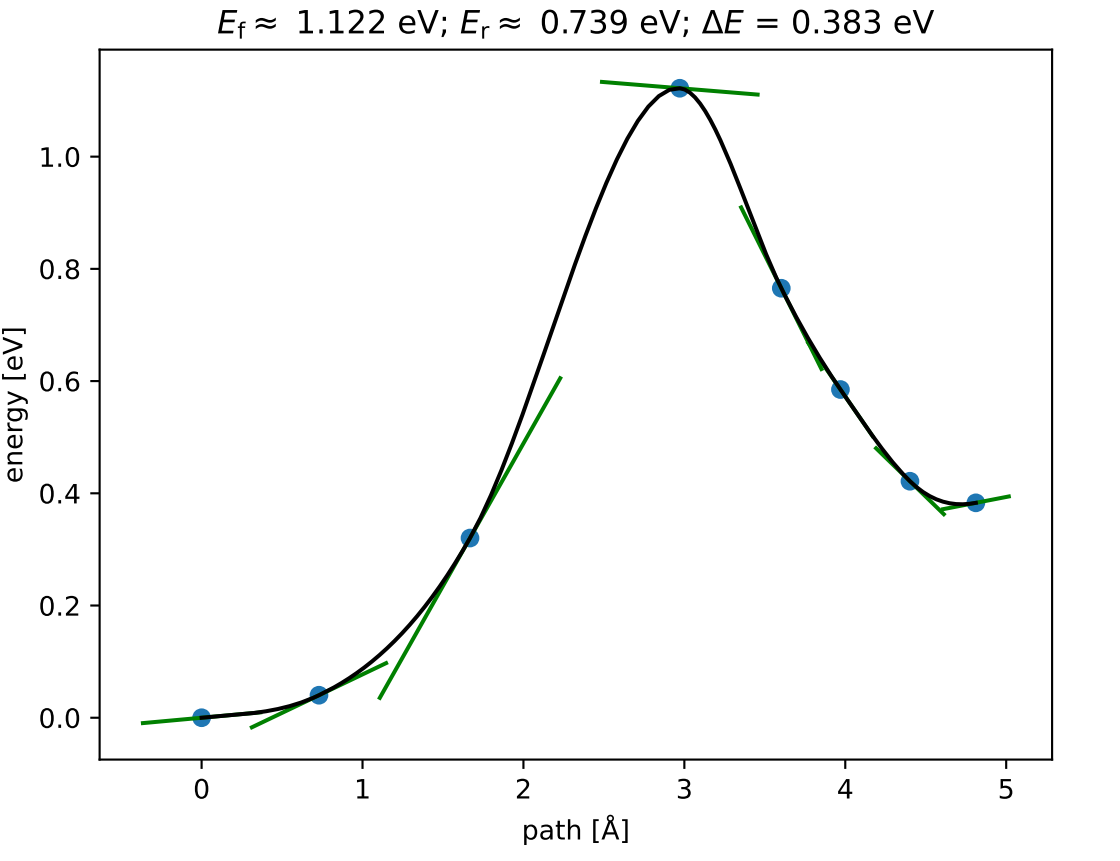
$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
energy [eV]
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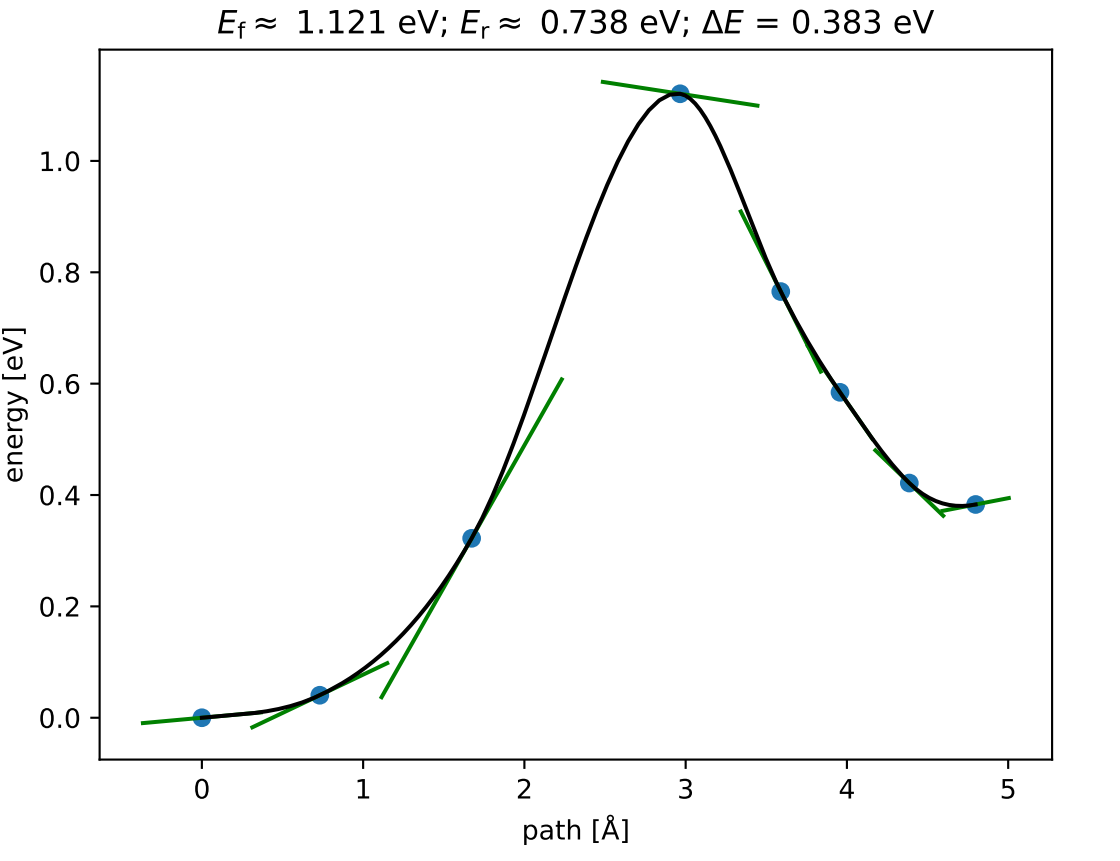
$E_f \approx$ 1.121 eV; $E_r \approx$ 0.738 eV; ΔE = 0.383 eV
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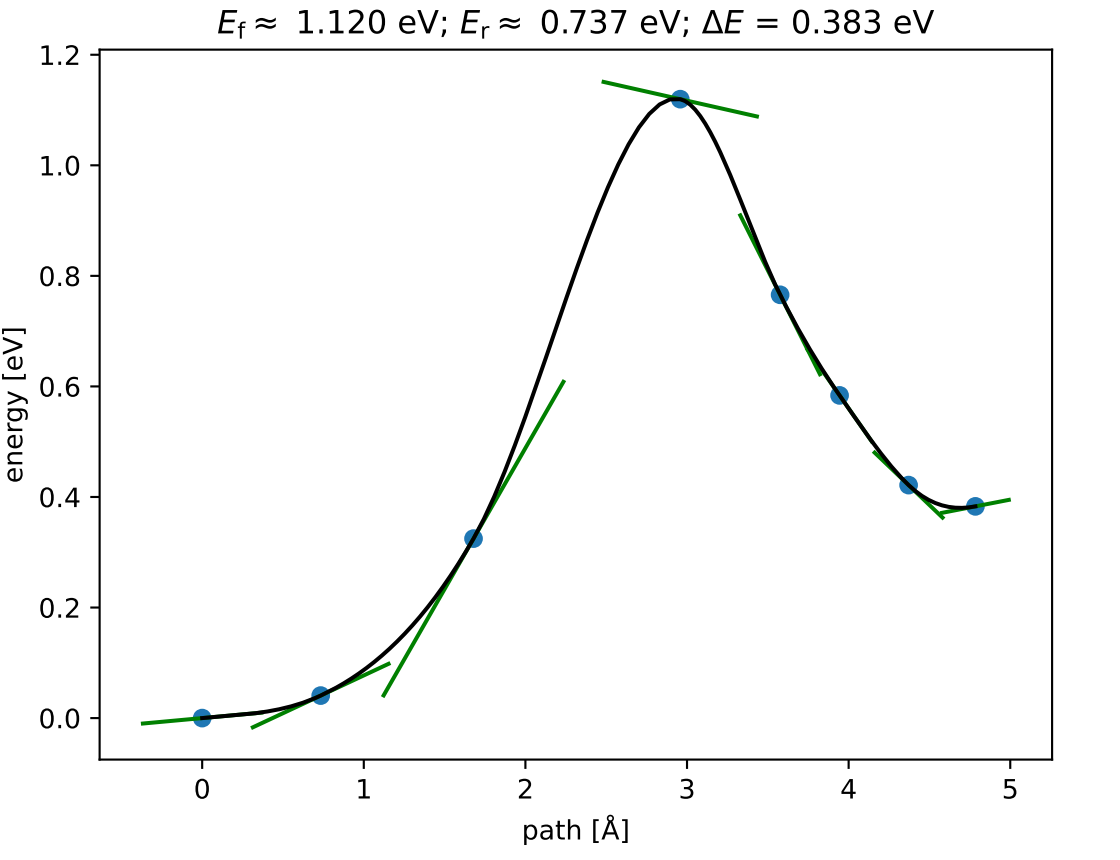
$E_f \approx$ 1.120 eV; $E_r \approx$ 0.737 eV; ΔE = 0.383 eV
energy [eV]
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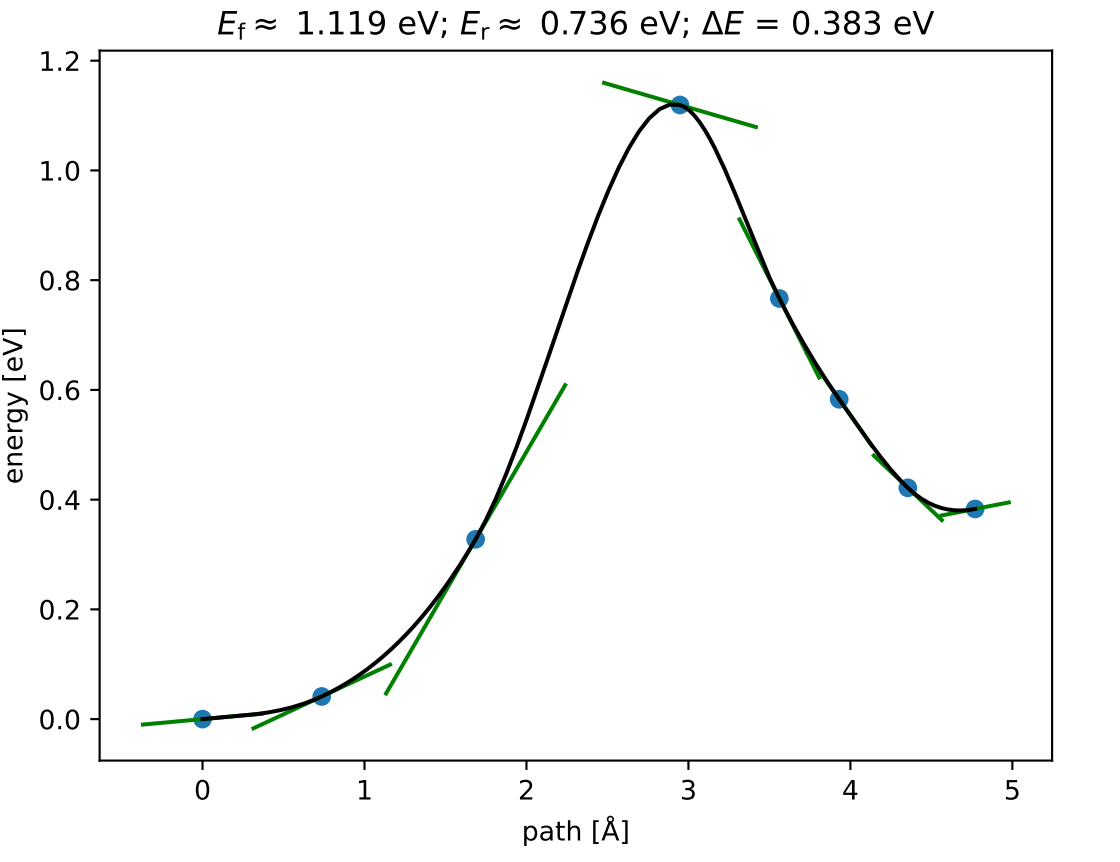
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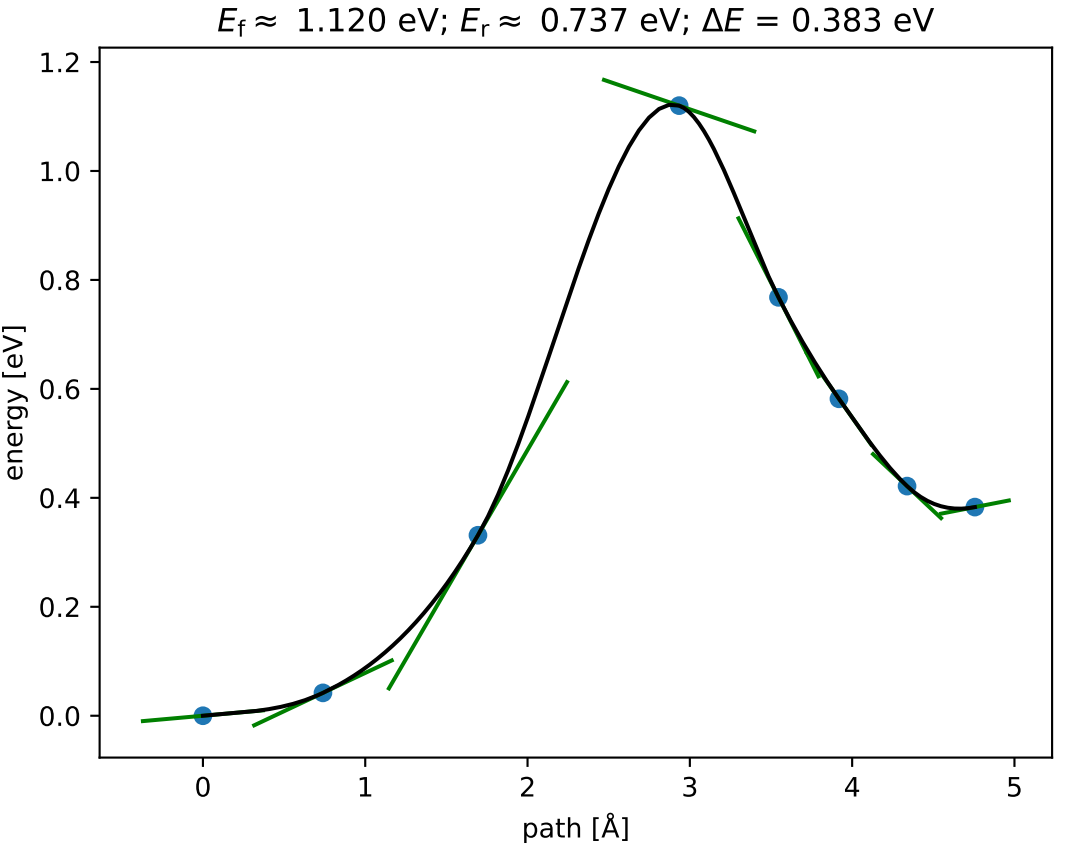
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energy [eV]
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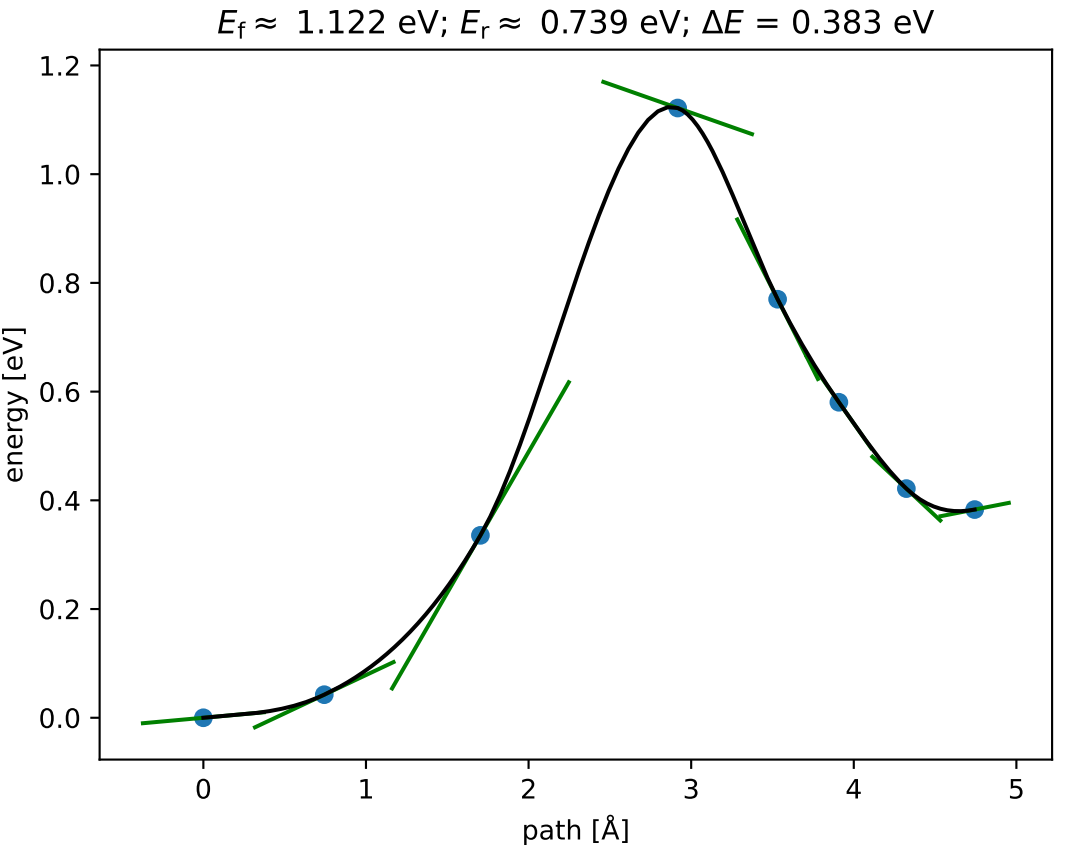
$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
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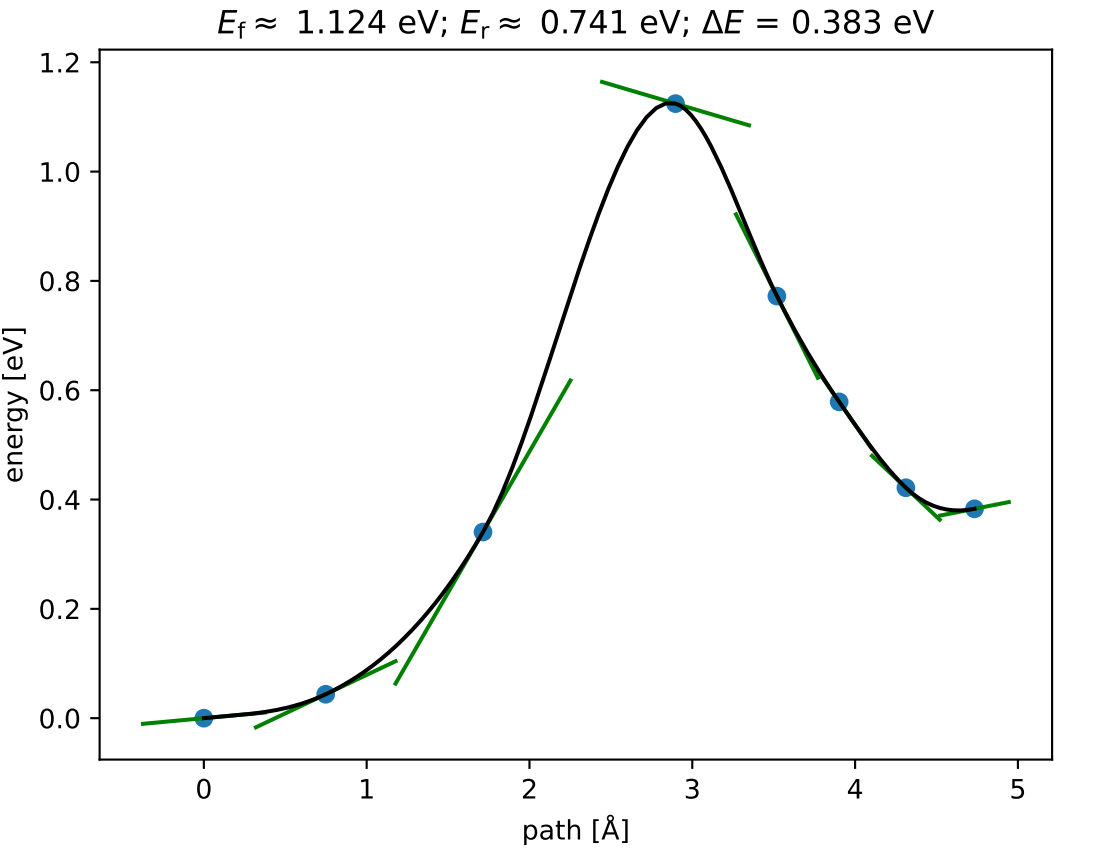
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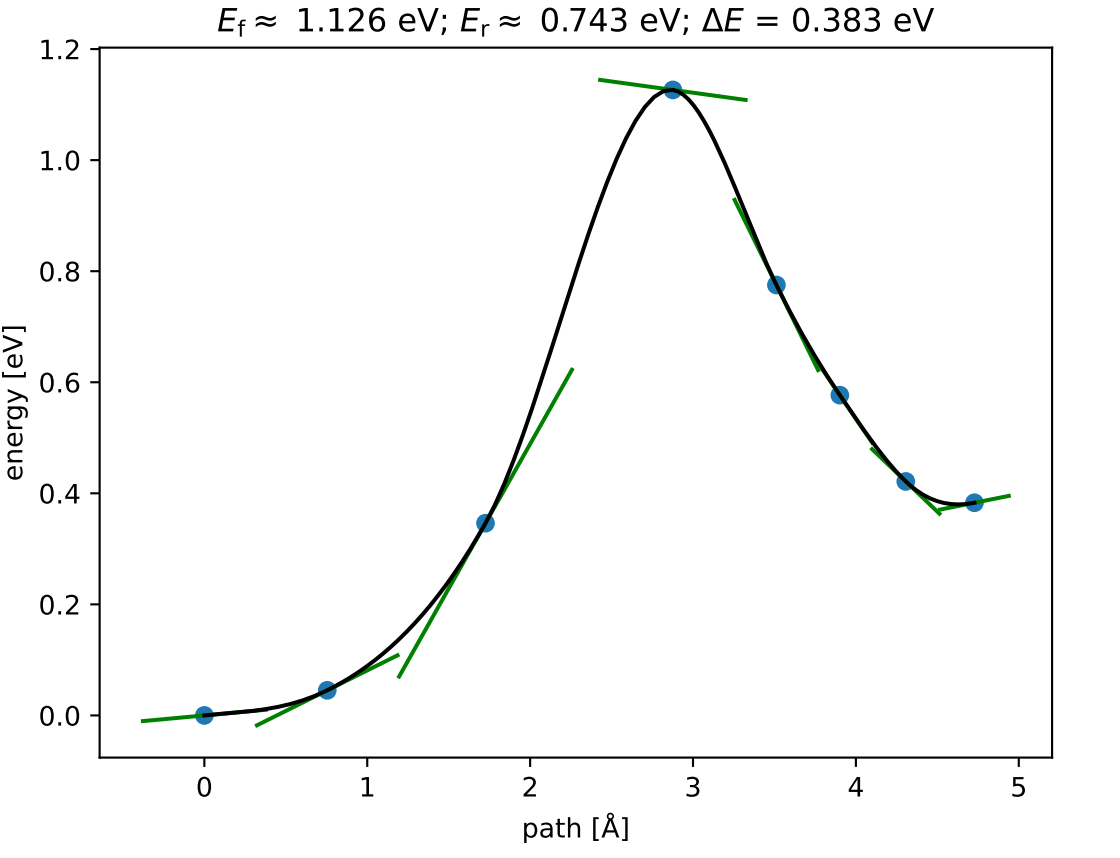
$E_f \approx$ 1.126 eV; $E_r \approx$ 0.743 eV; ΔE = 0.383 eV
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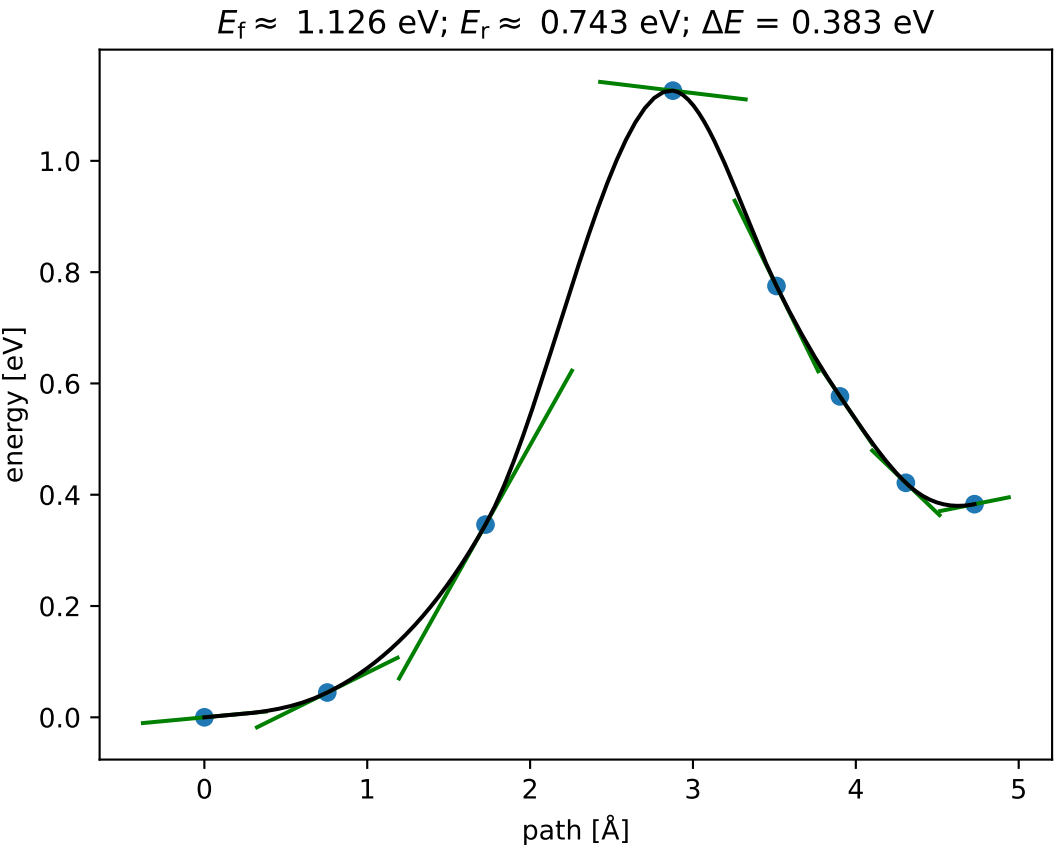
$E_f \approx$ 1.126 eV; $E_r \approx$ 0.743 eV; ΔE = 0.383 eV
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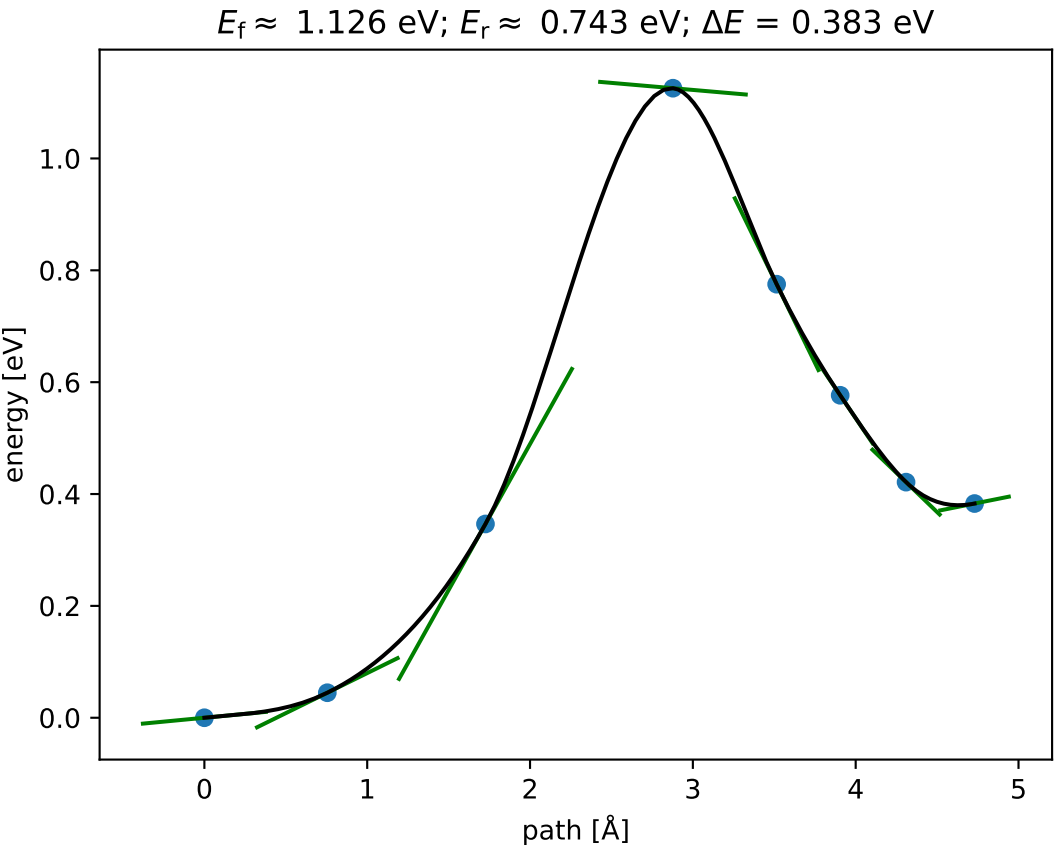
$E_f \approx$ 1.126 eV; $E_r \approx$ 0.743 eV; ΔE = 0.383 eV
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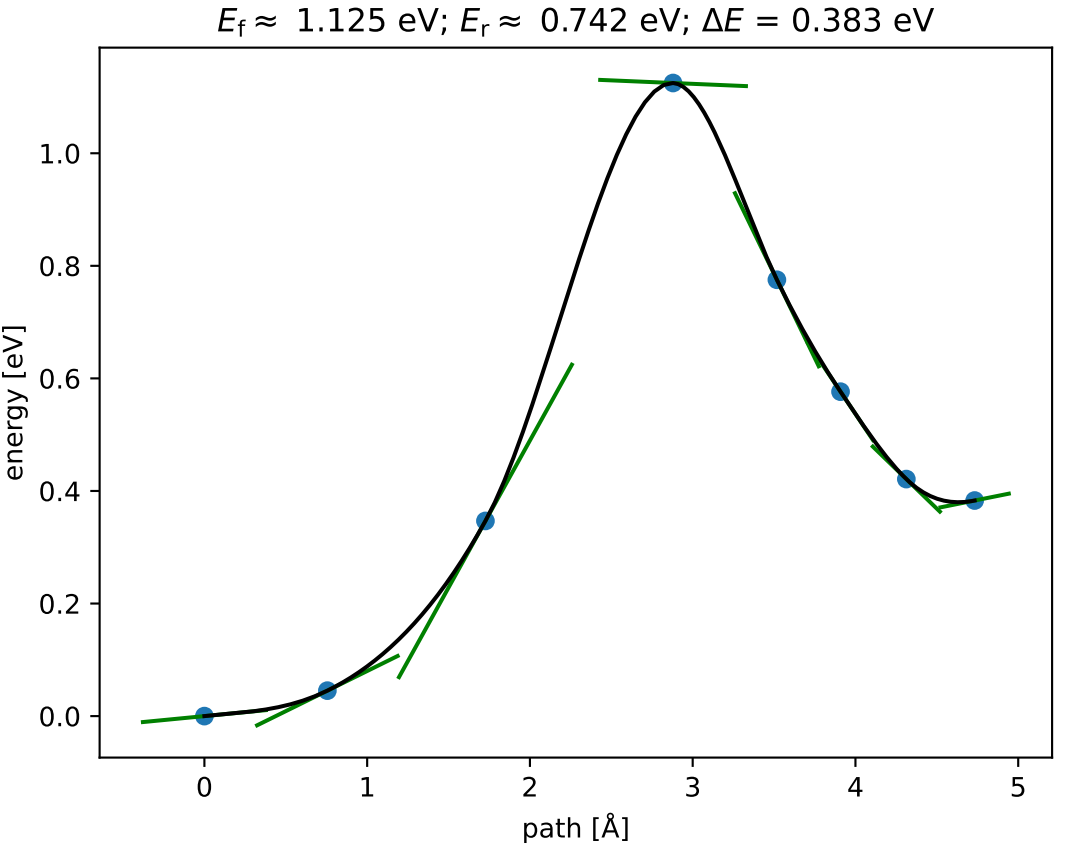
$E_f \approx$ 1.125 eV; $E_r \approx$ 0.742 eV; ΔE = 0.383 eV
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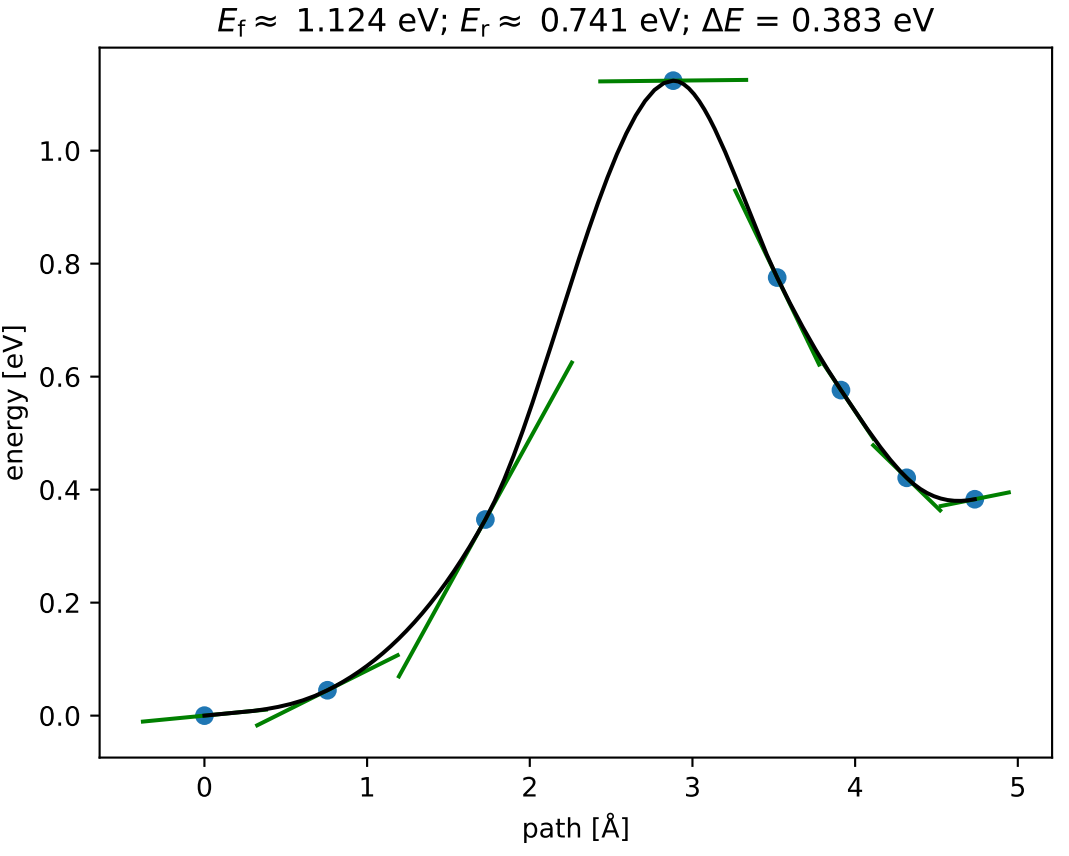
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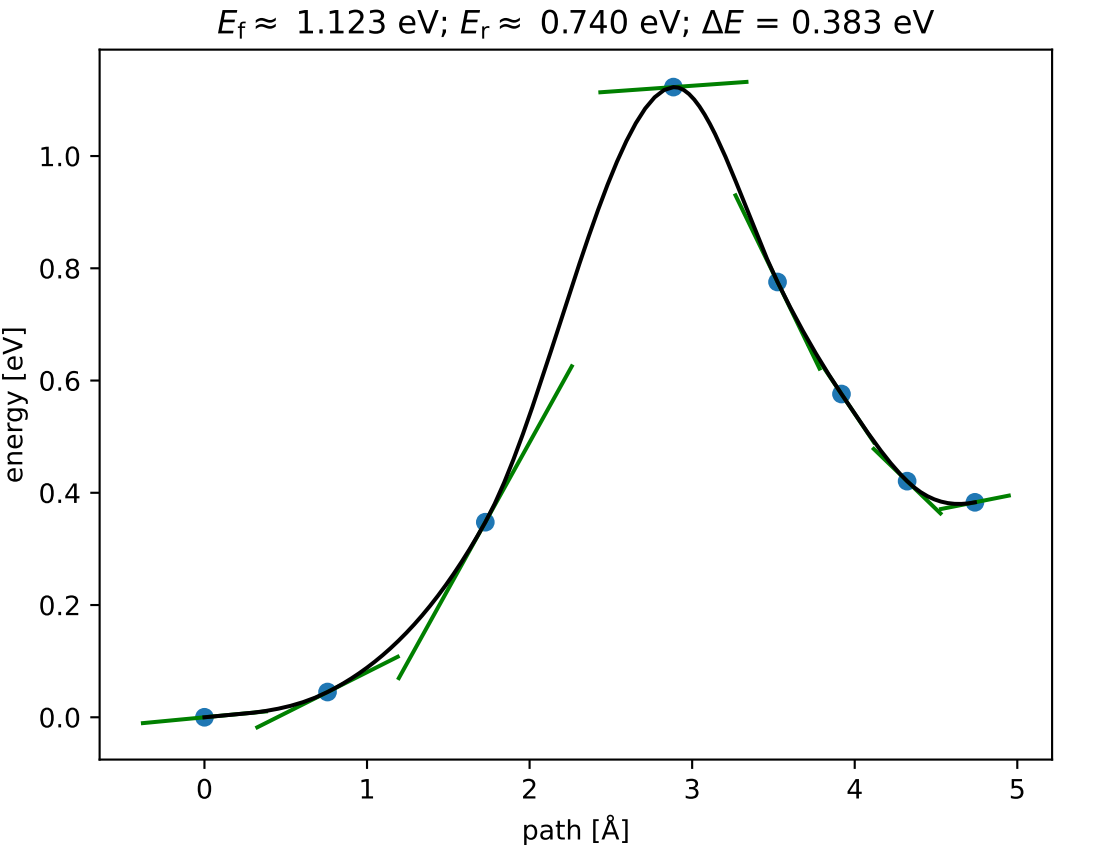
$E_f \approx$ 1.123 eV; $E_r \approx$ 0.740 eV; ΔE = 0.383 eV
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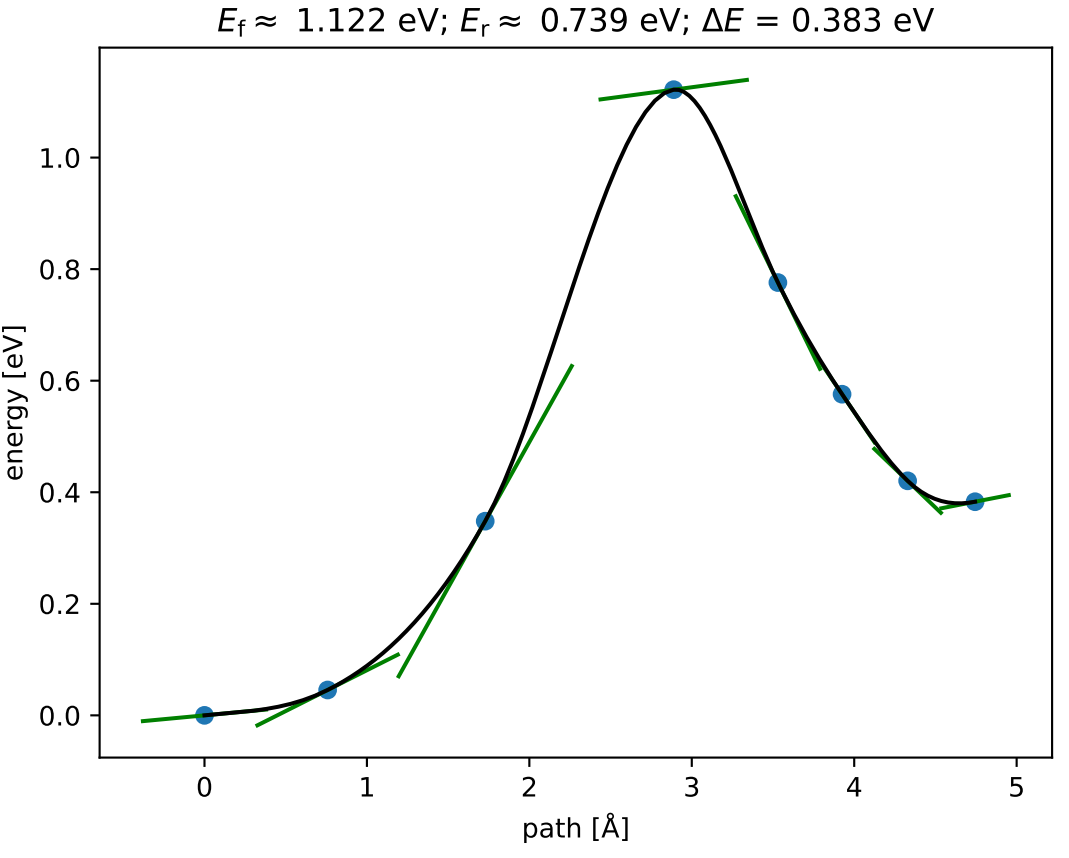
$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 eV; ΔE = 0.383 eV
energy [eV]
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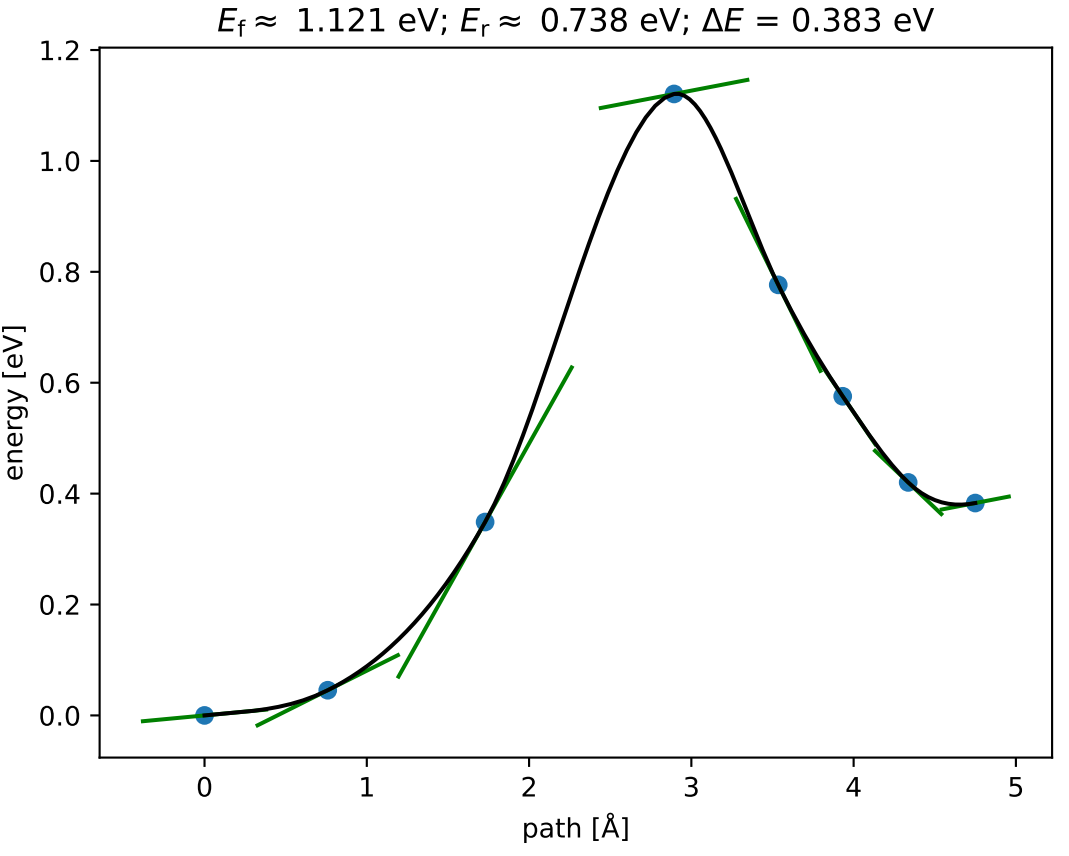
$E_f \approx$ 1.121 eV; $E_r \approx$ 0.738 eV; ΔE = 0.383 eV
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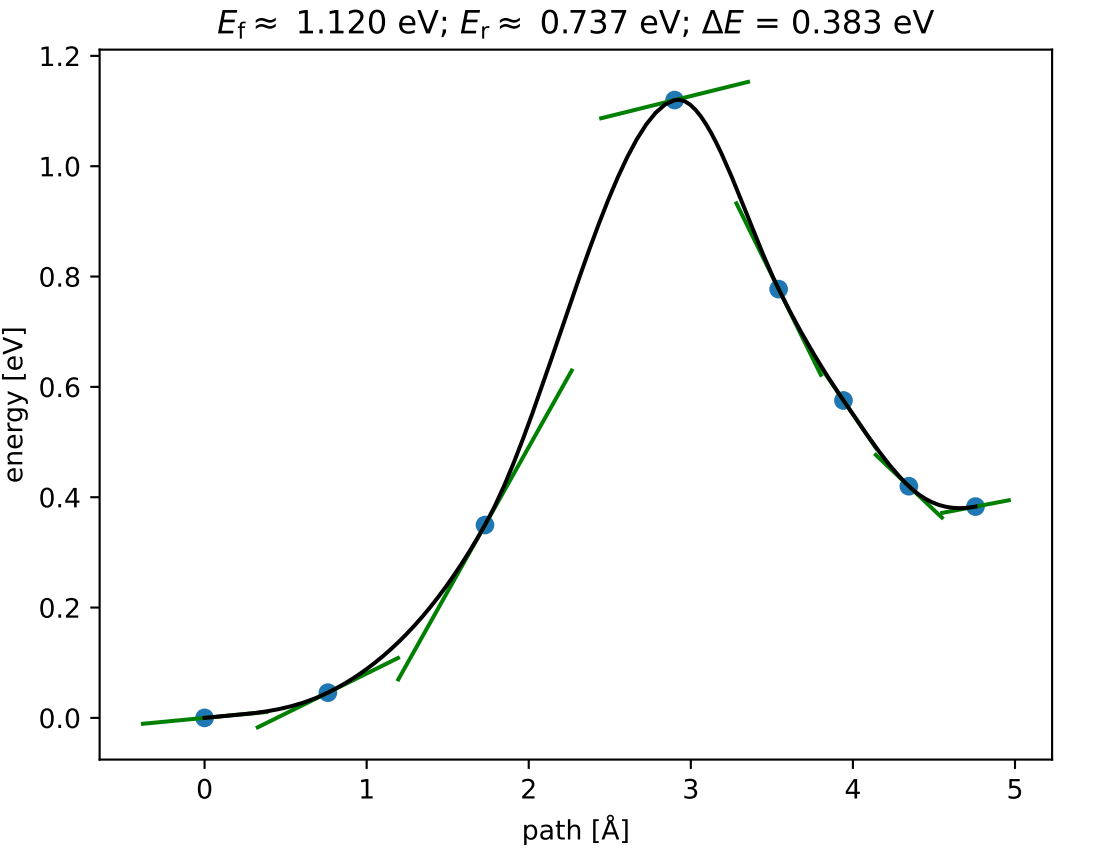
$E_f \approx$ 1.120 eV; $E_r \approx$ 0.737 eV; ΔE = 0.383 eV
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path [Å]
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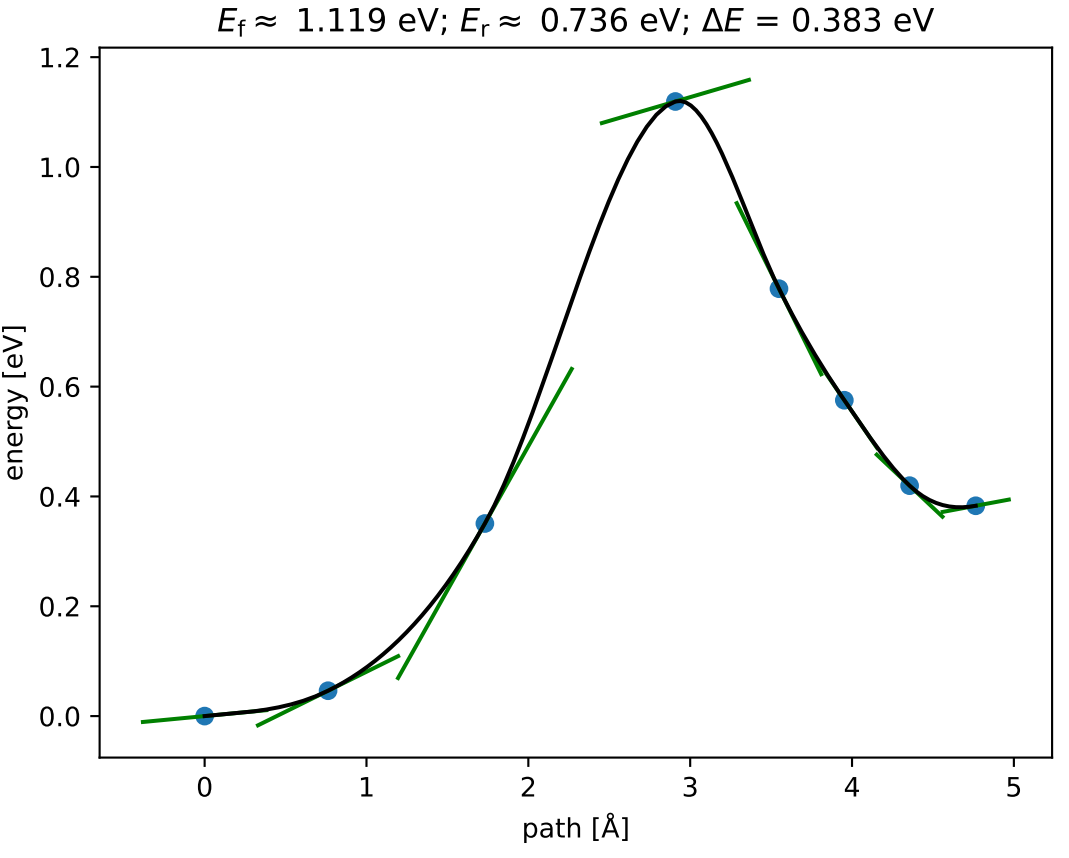
$E_f \approx$ 1.119 eV; $E_r \approx$ 0.736 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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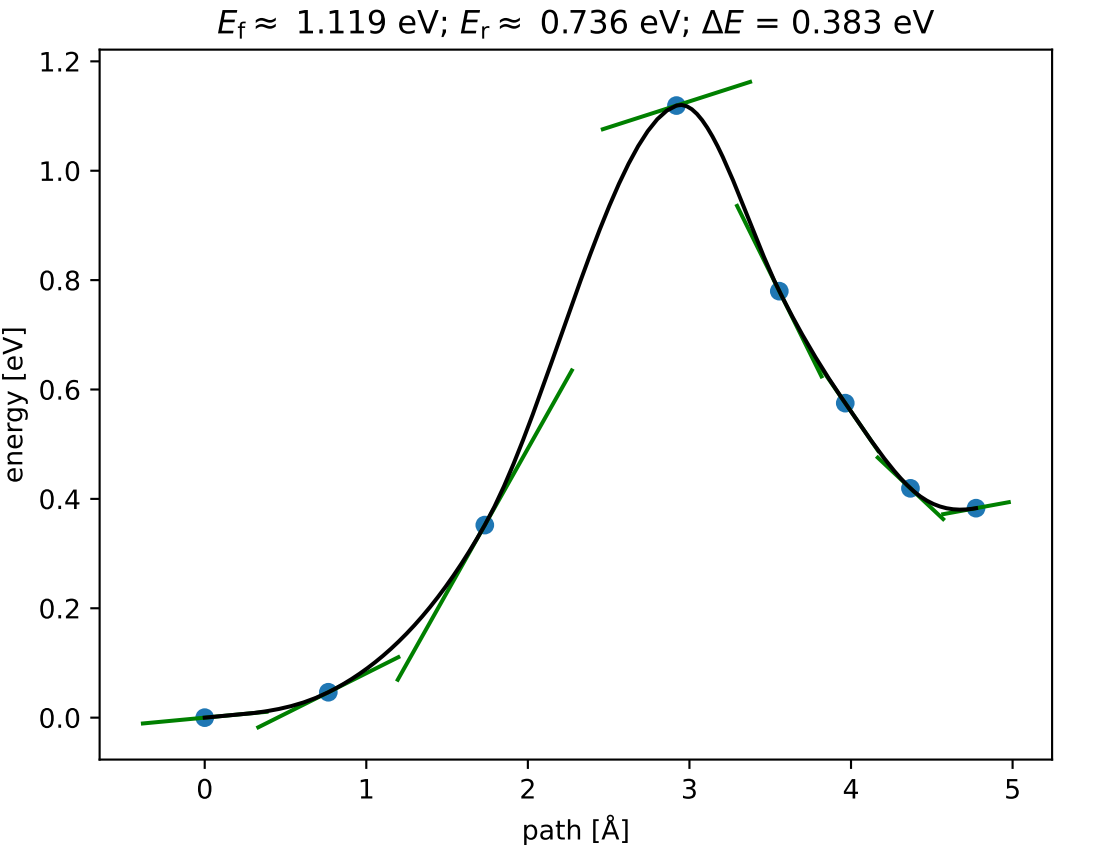
$E_f \approx$ 1.119 eV; $E_r \approx$ 0.736 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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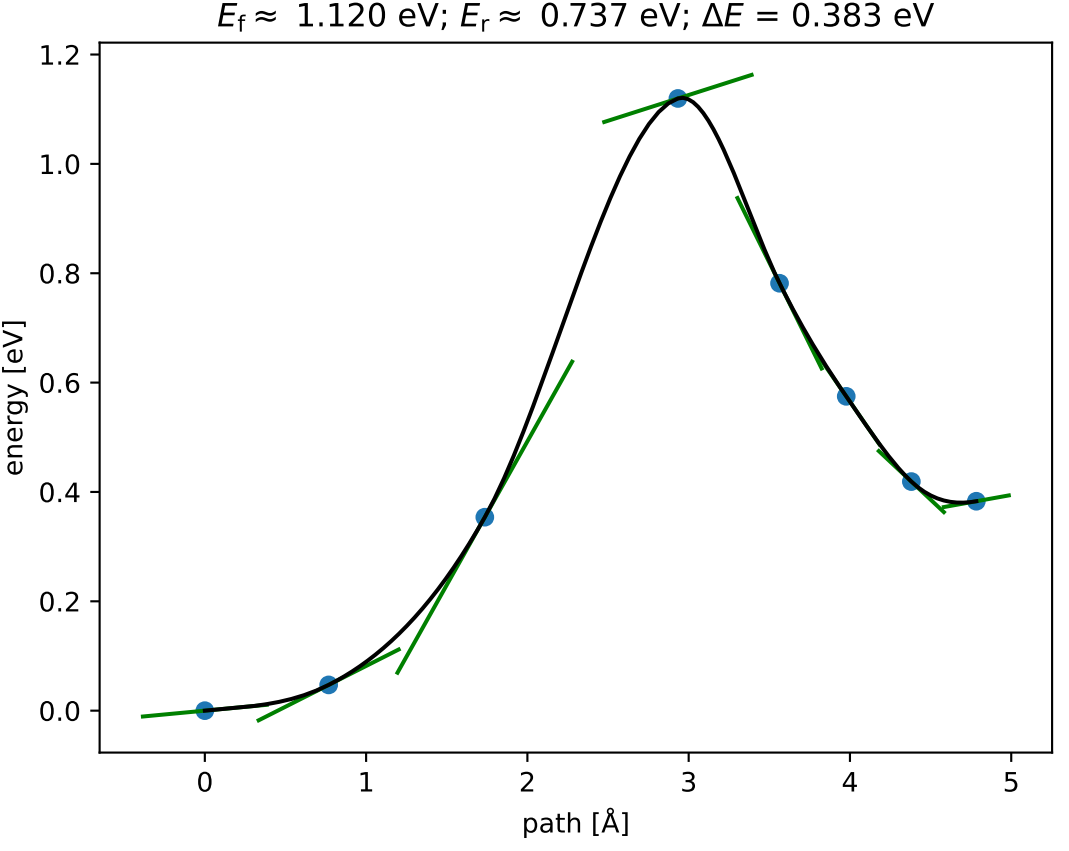
3
4
5


$E_f \approx$ 1.120 eV; $E_r \approx$ 0.737 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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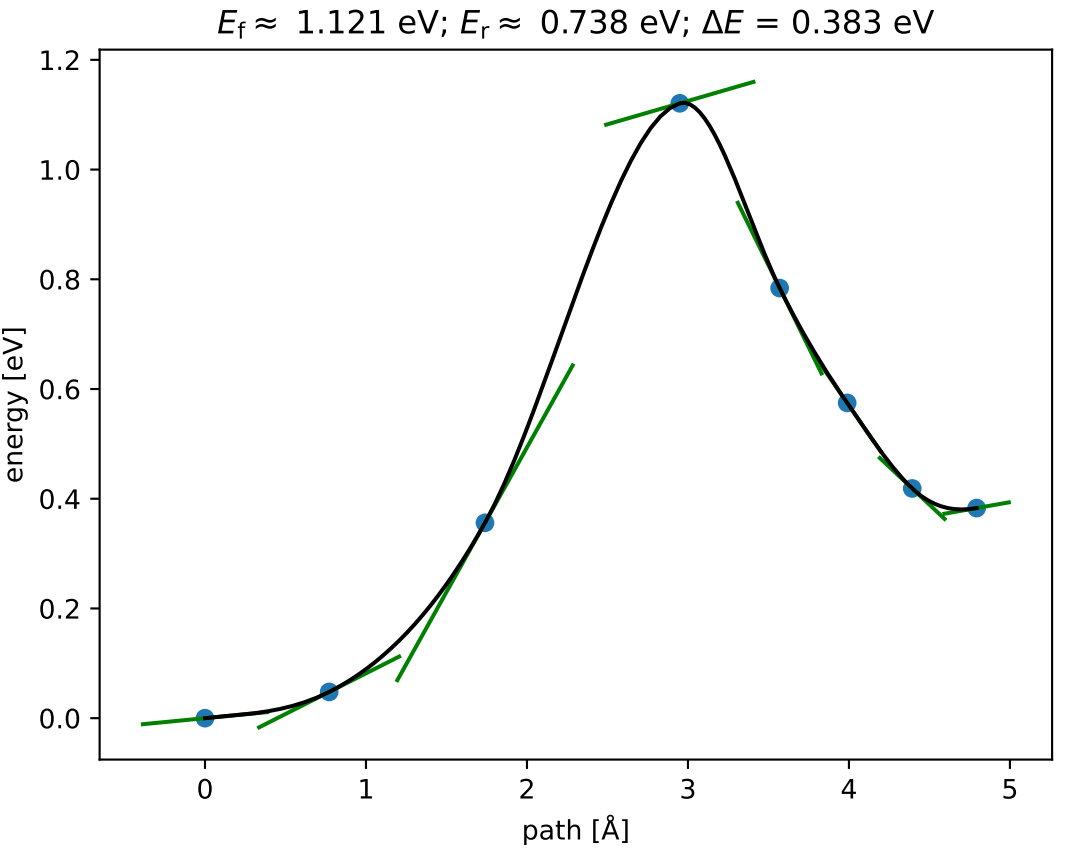
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.121 eV; $E_r \approx$ 0.738 eV; ΔE = 0.383 eV
energy [eV]
path [Å]
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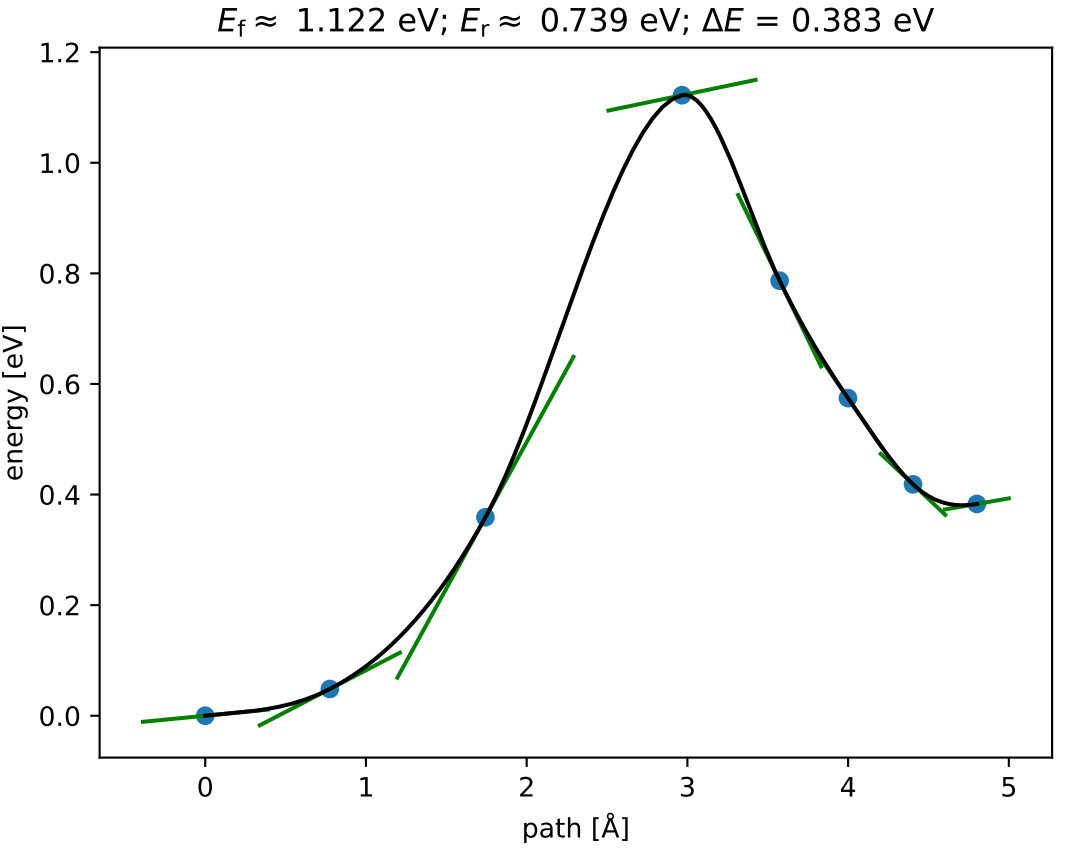
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5


$E_f \approx$ 1.122 eV; $E_r \approx$ 0.739 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