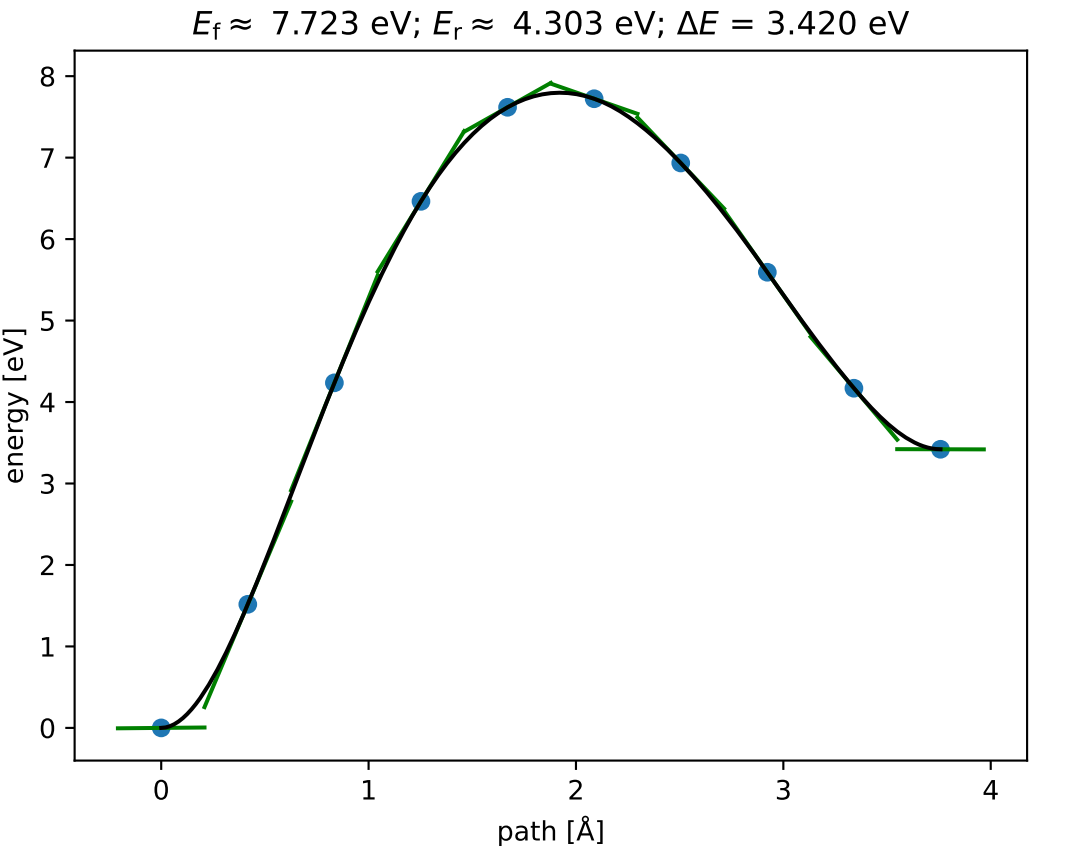
$E_f \approx$ 7.723 eV; $E_r \approx$ 4.303 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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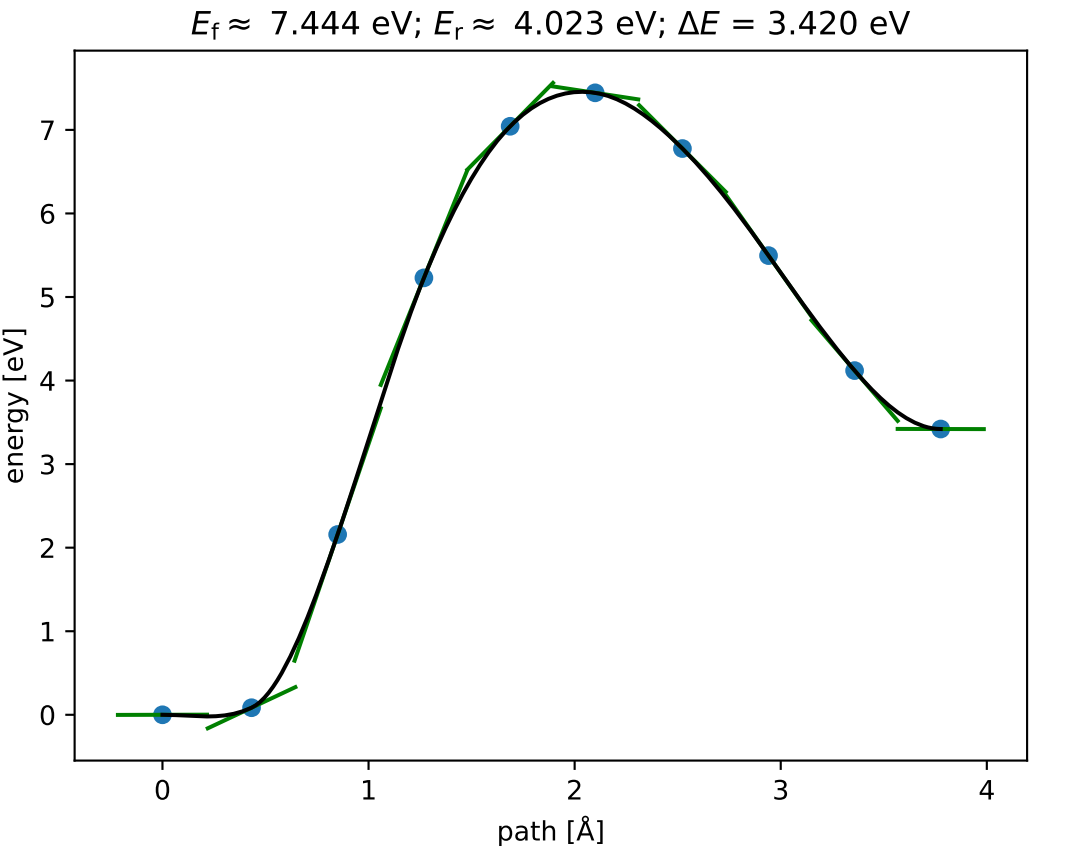
$E_f \approx$ 7.444 eV; $E_r \approx$ 4.023 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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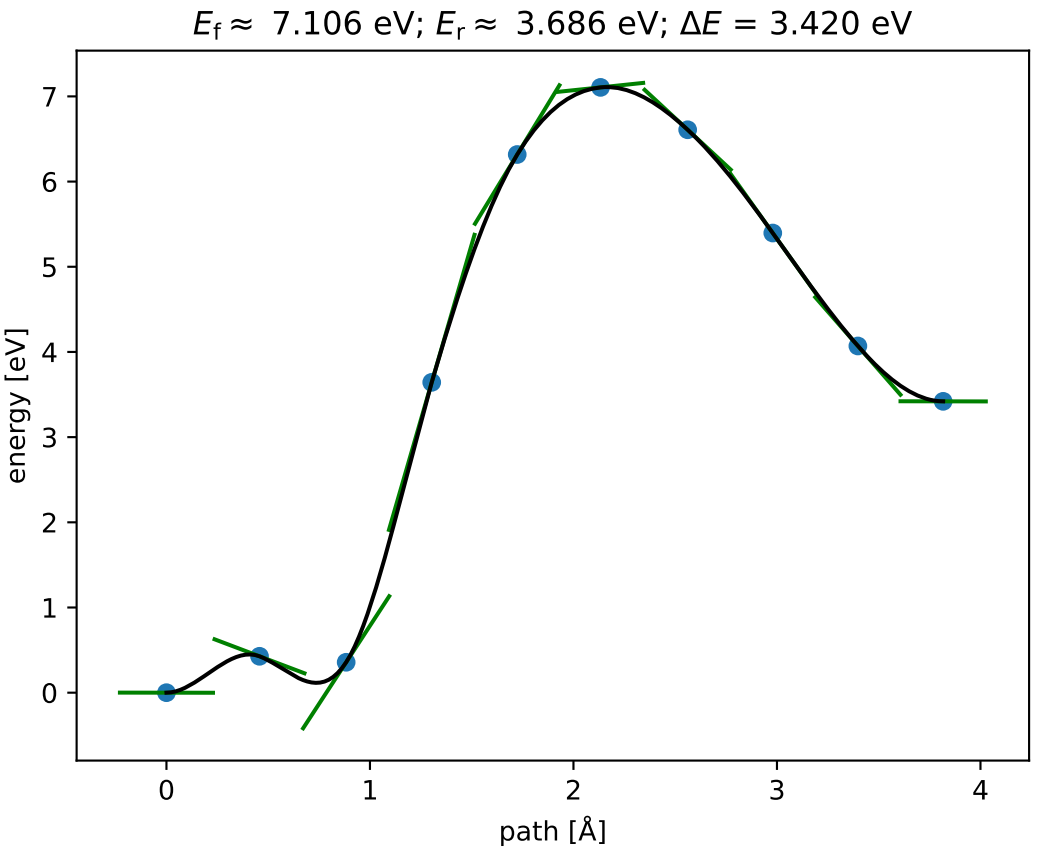
$E_f \approx$ 7.106 eV; $E_r \approx$ 3.686 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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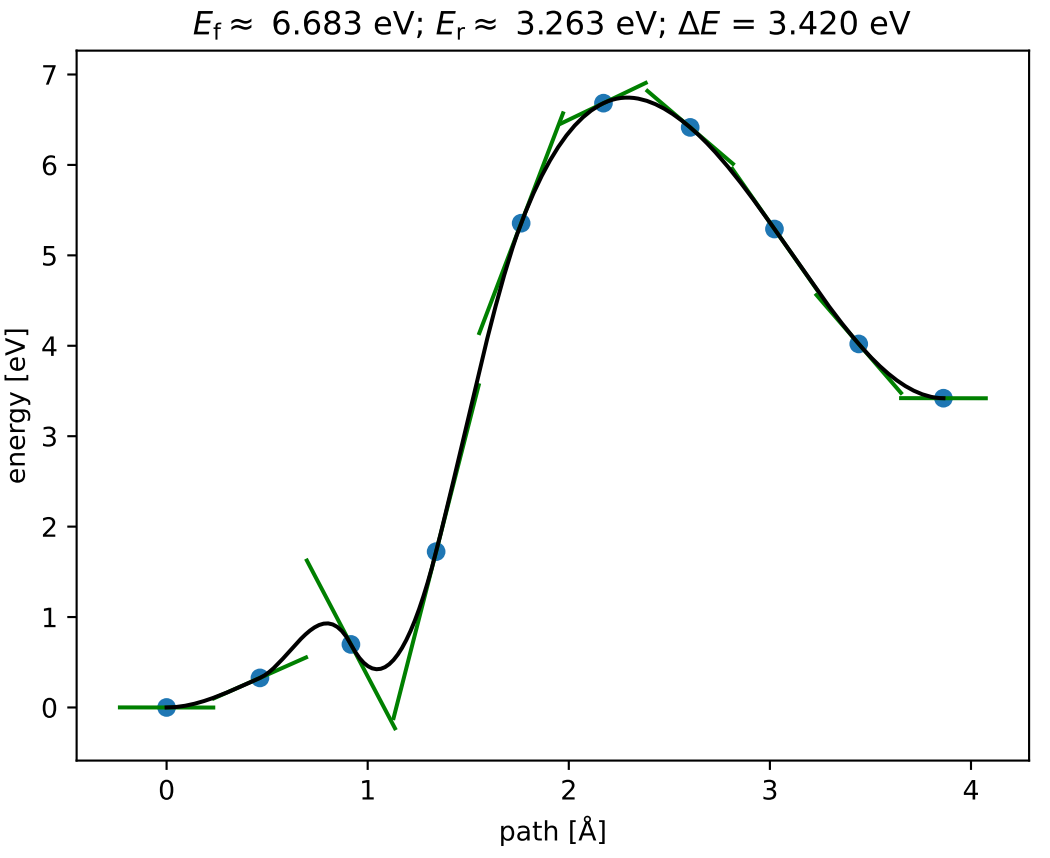
$E_f \approx$ 6.683 eV; $E_r \approx$ 3.263 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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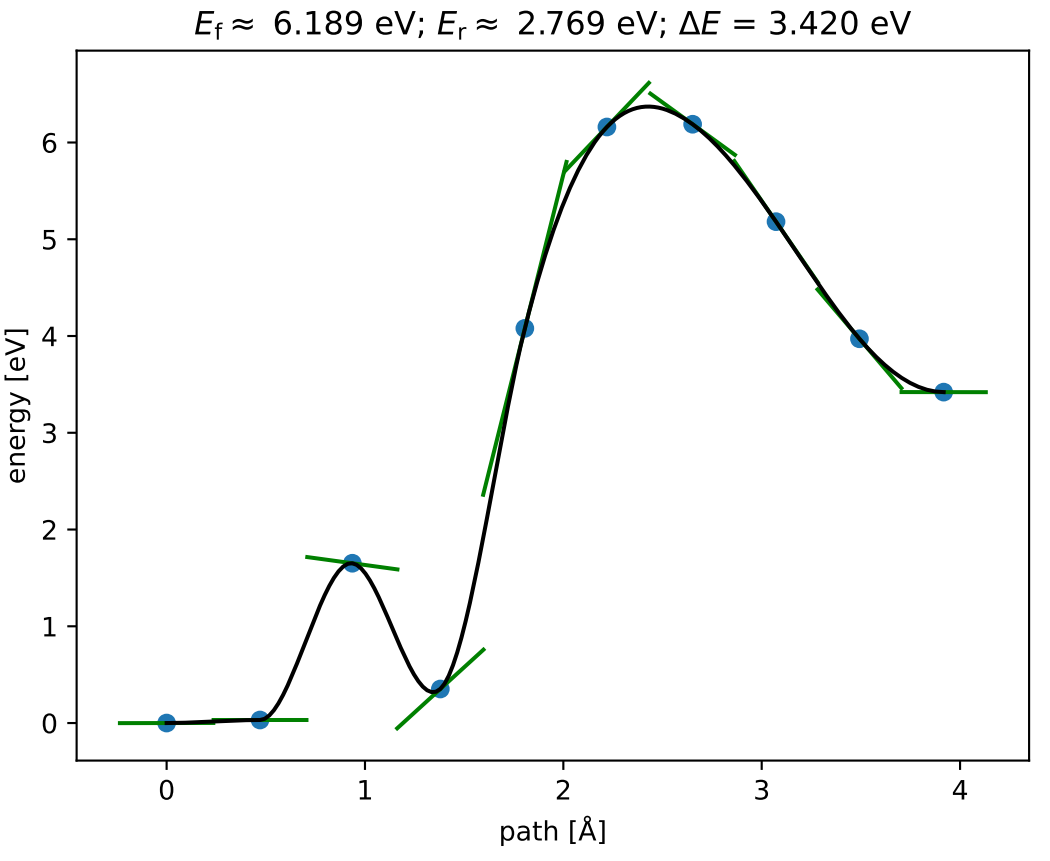
$E_f \approx$ 6.189 eV; $E_r \approx$ 2.769 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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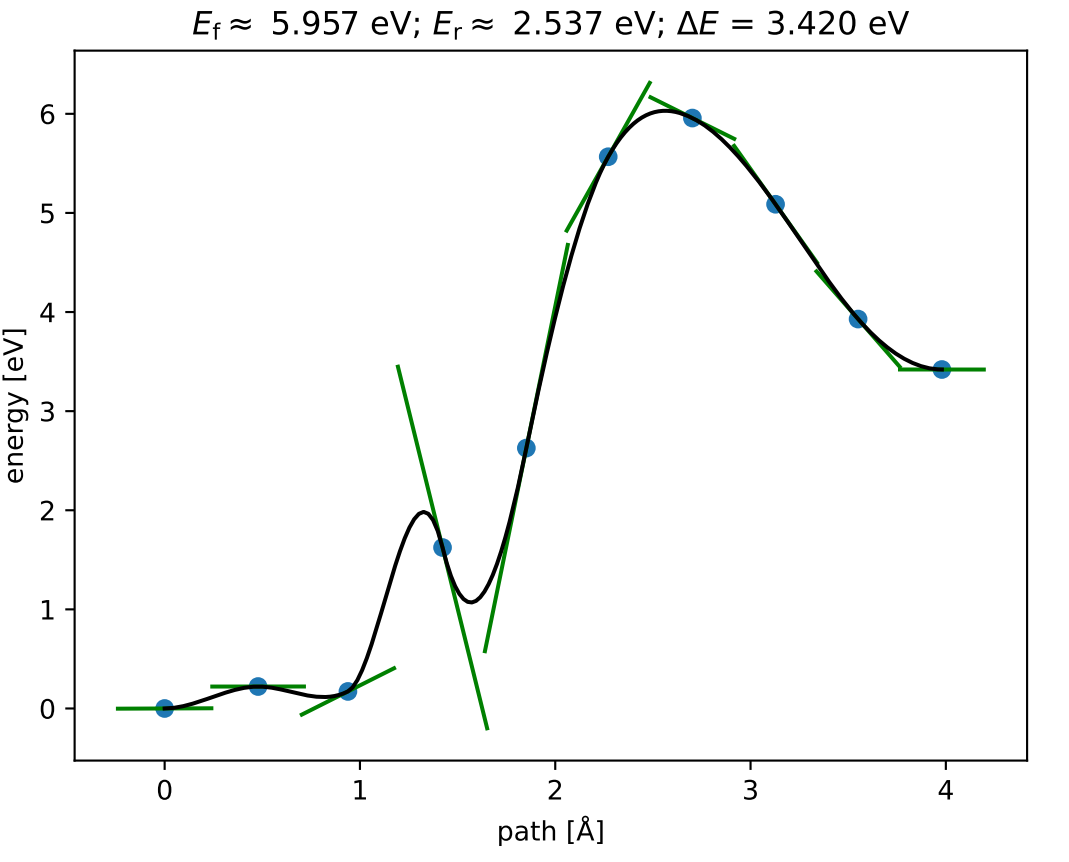
$E_f \approx$ 5.957 eV; $E_r \approx$ 2.537 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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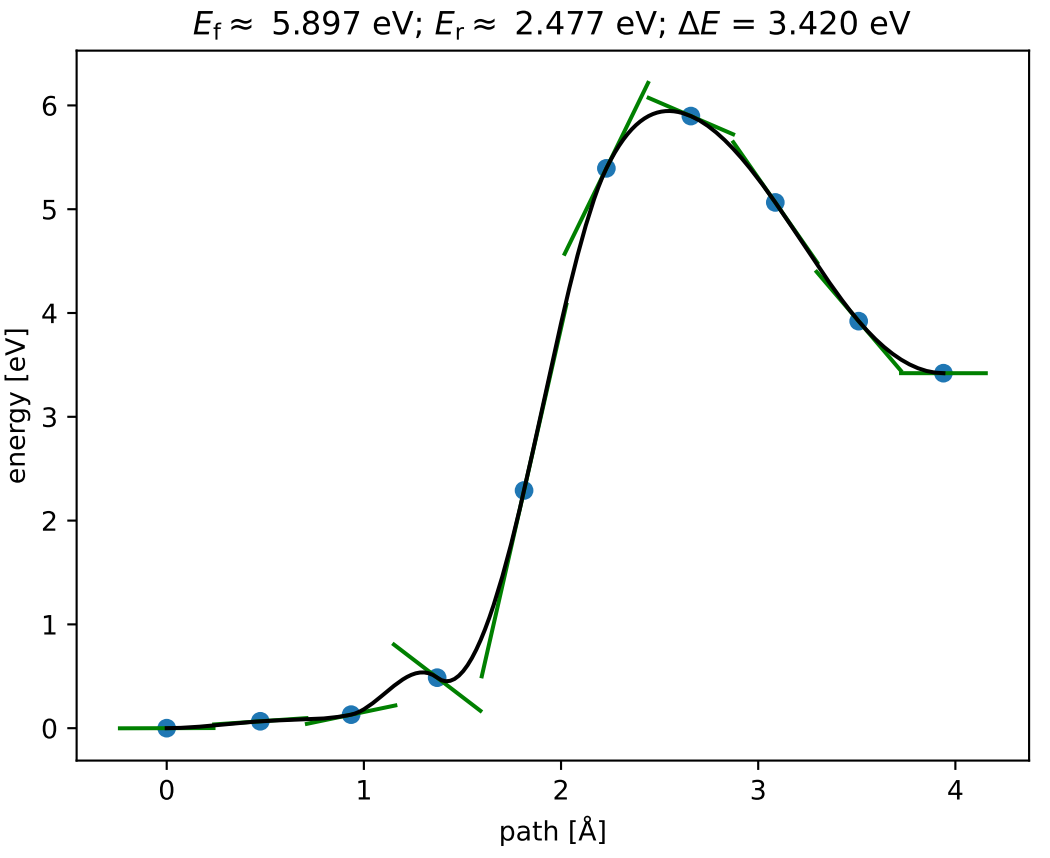
$E_f \approx$ 5.897 eV; $E_r \approx$ 2.477 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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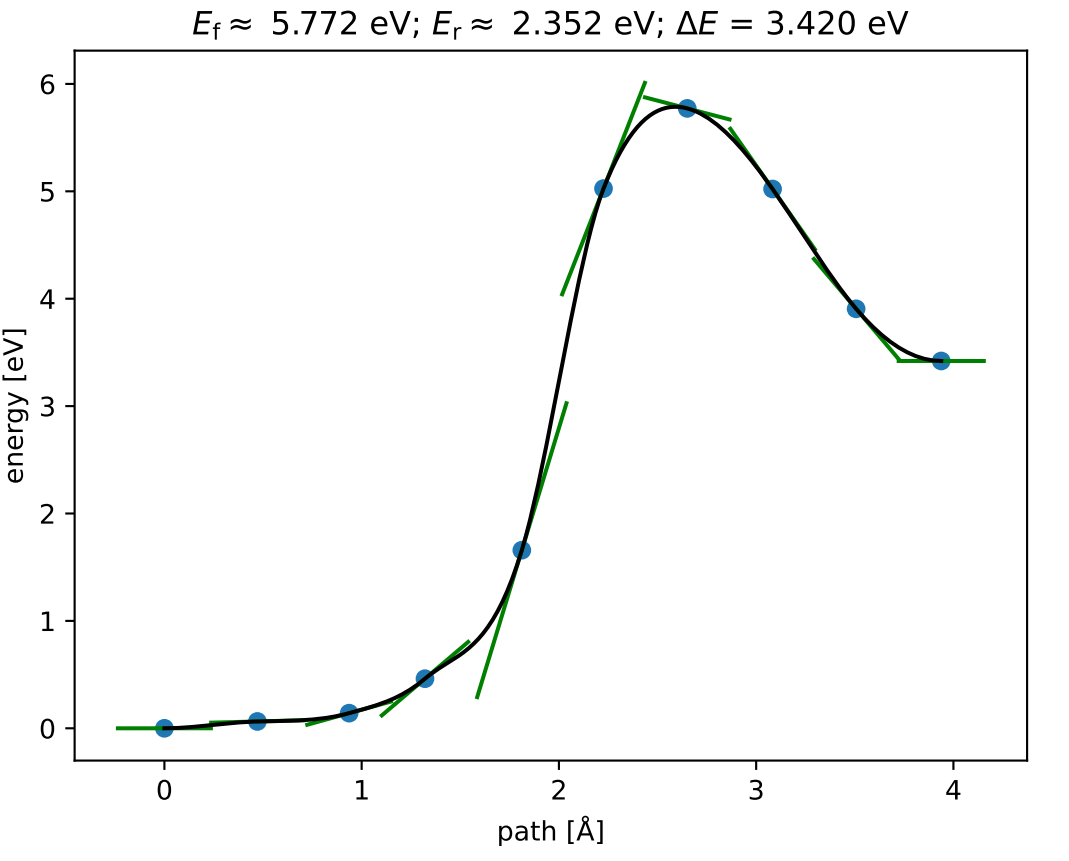
$E_f \approx$ 5.772 eV; $E_r \approx$ 2.352 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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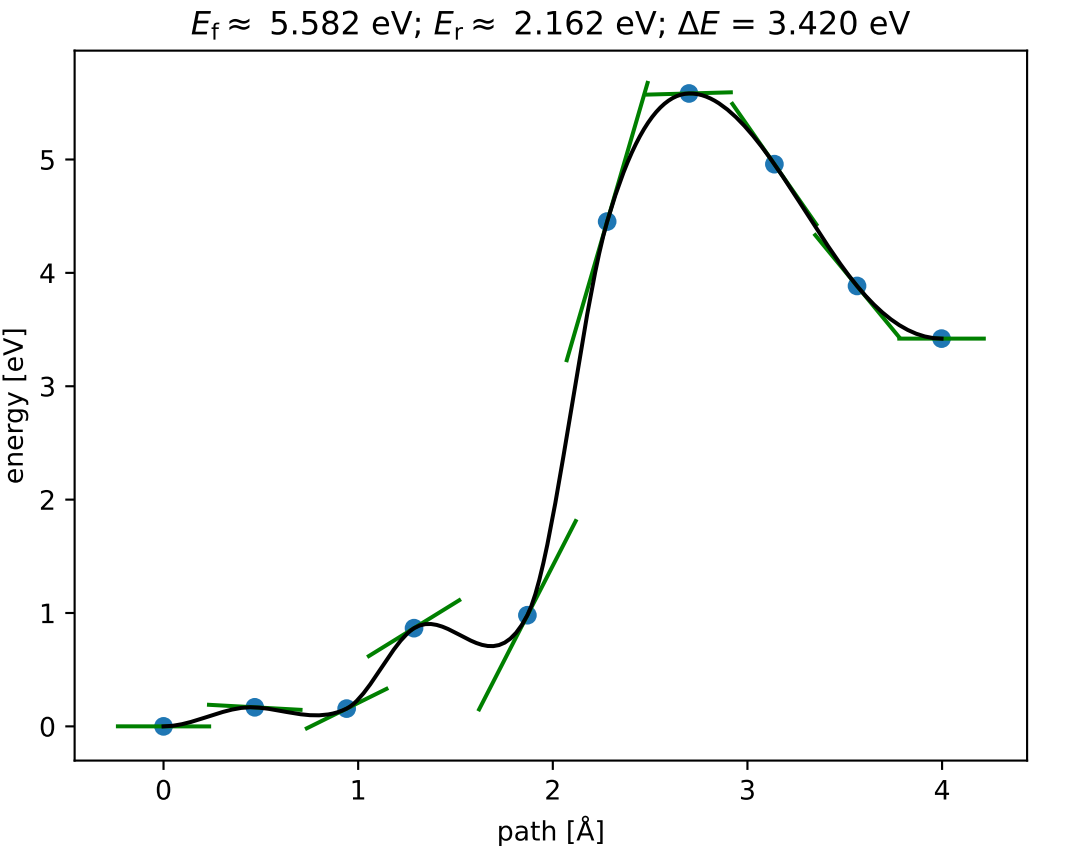
$E_f \approx$ 5.582 eV; $E_r \approx$ 2.162 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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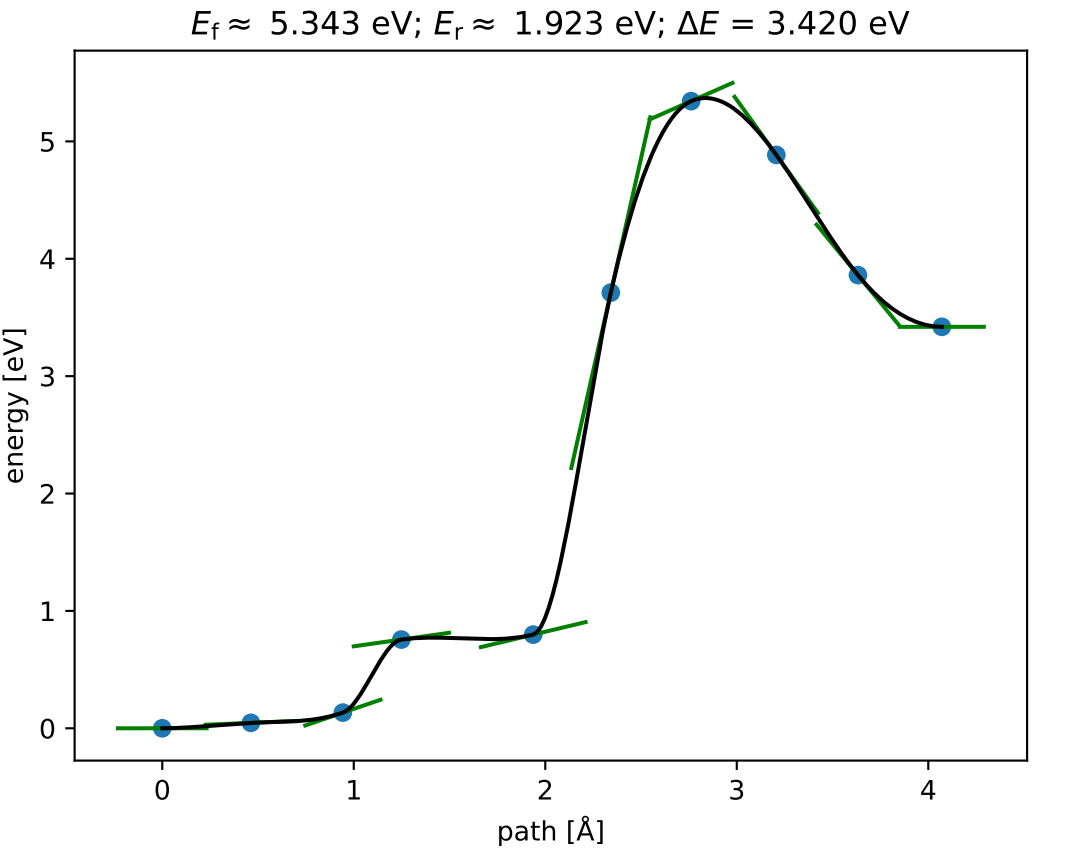
$E_f \approx$ 5.343 eV; $E_r \approx$ 1.923 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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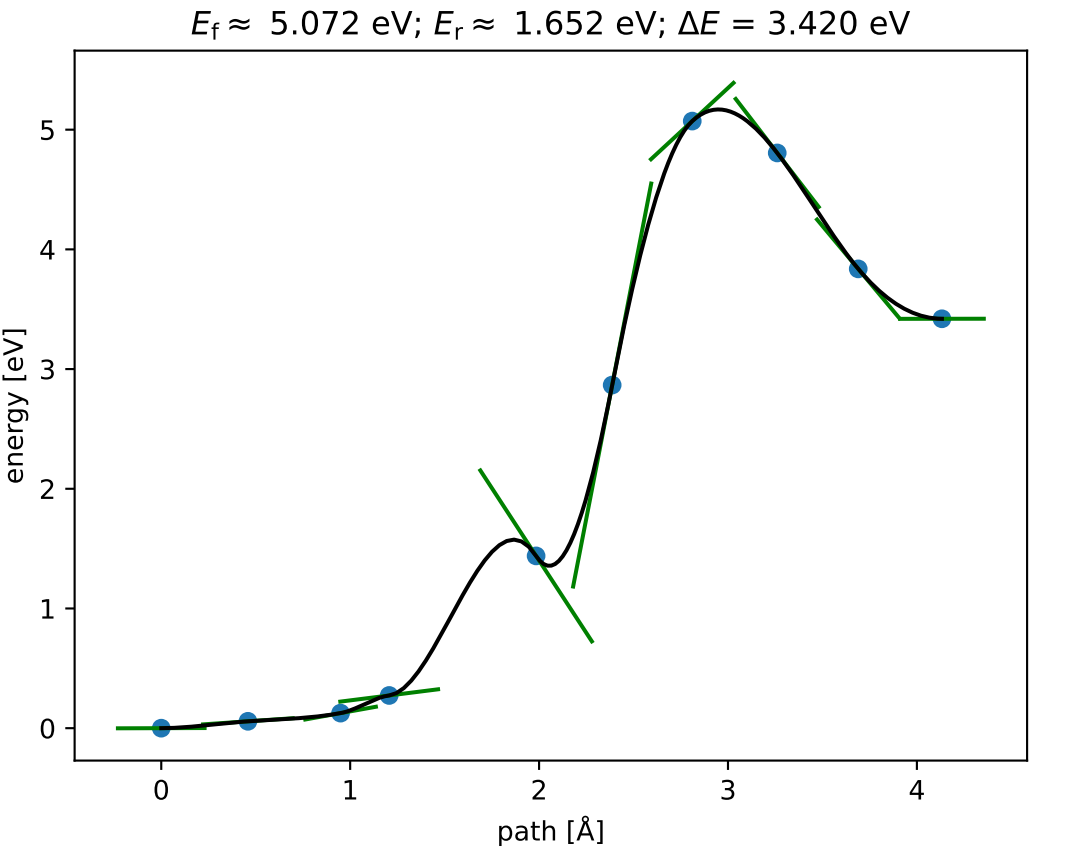
$E_f \approx$ 5.072 eV; $E_r \approx$ 1.652 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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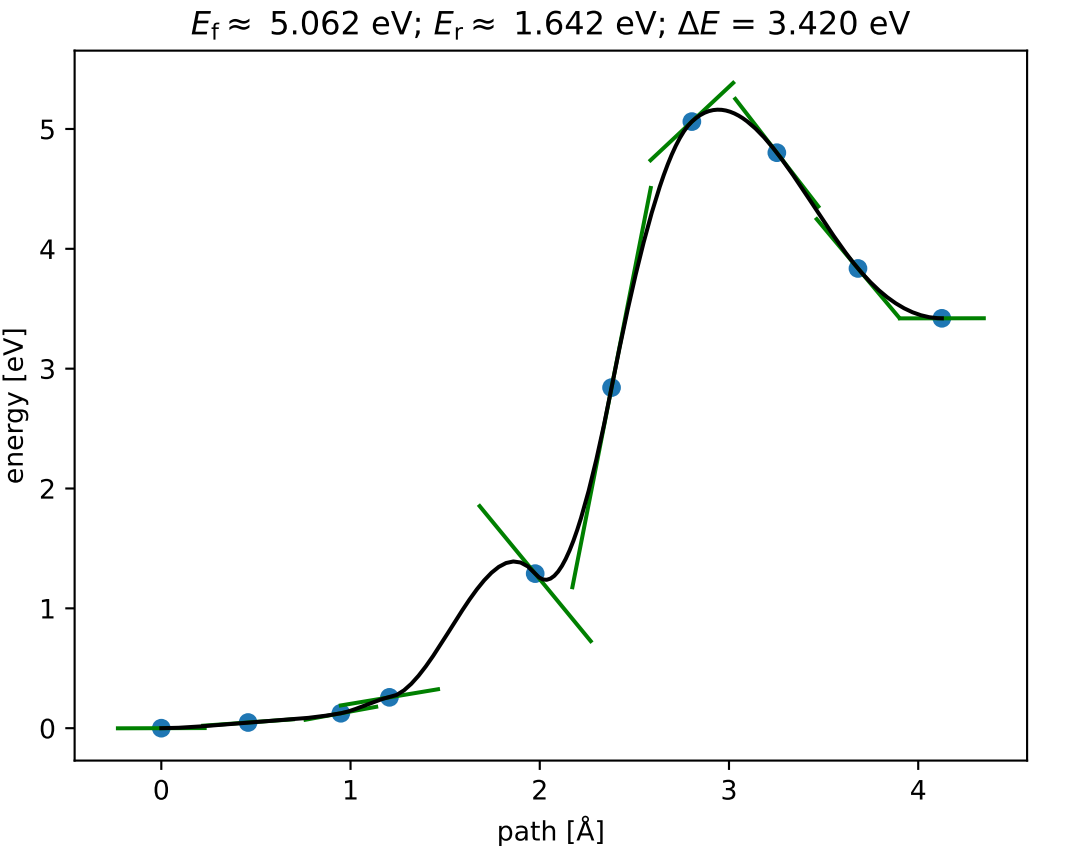
$E_f \approx$ 5.062 eV; $E_r \approx$ 1.642 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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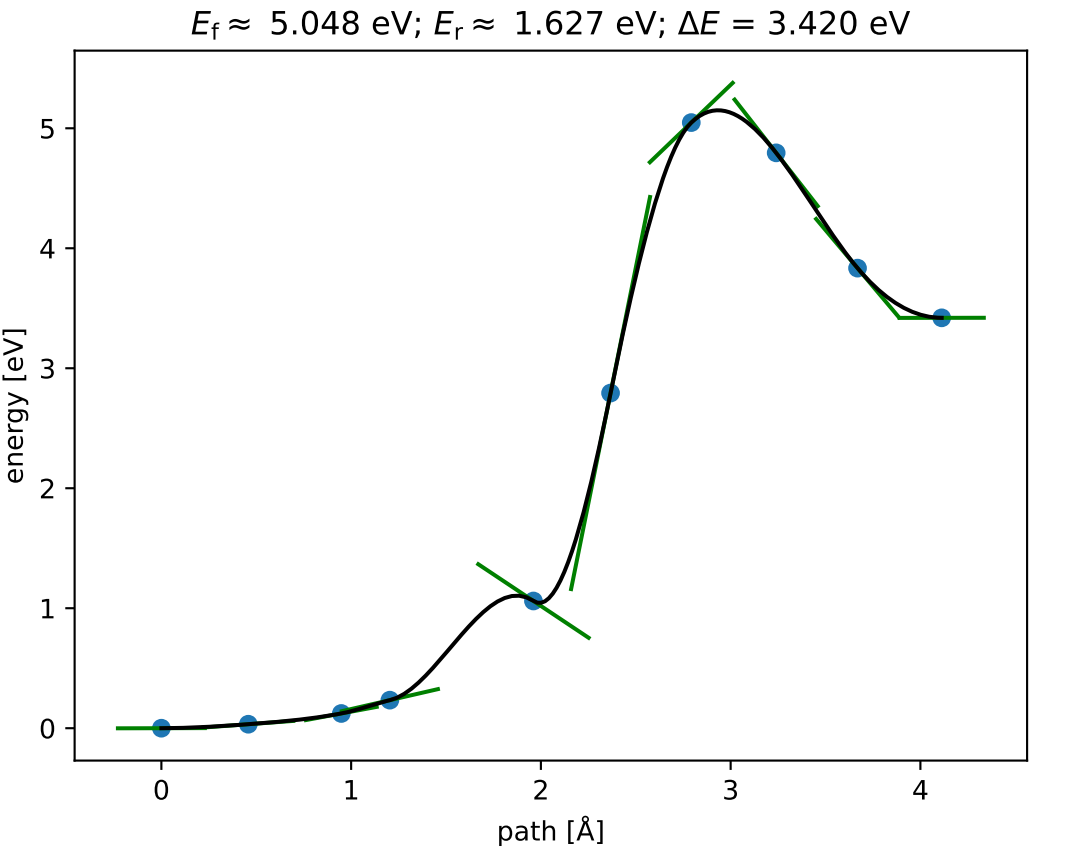
$E_f \approx$ 5.048 eV; $E_r \approx$ 1.627 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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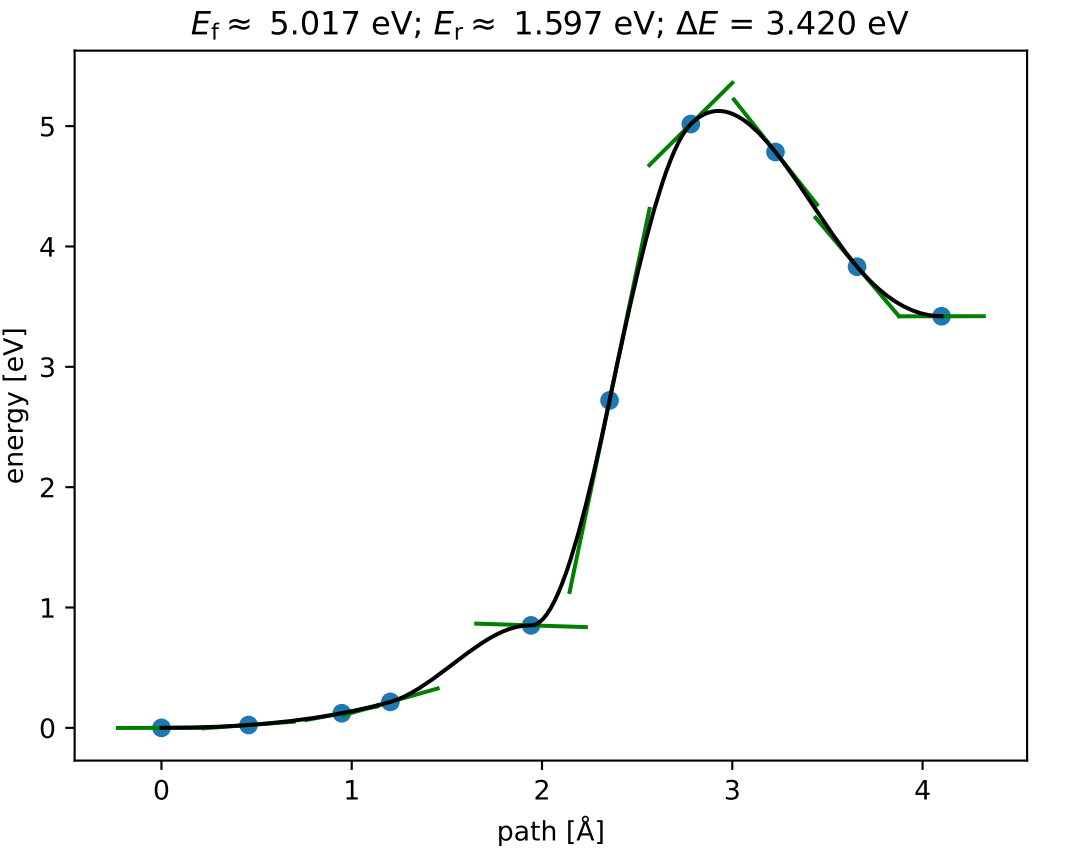
$E_f \approx$ 5.017 eV; $E_r \approx$ 1.597 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
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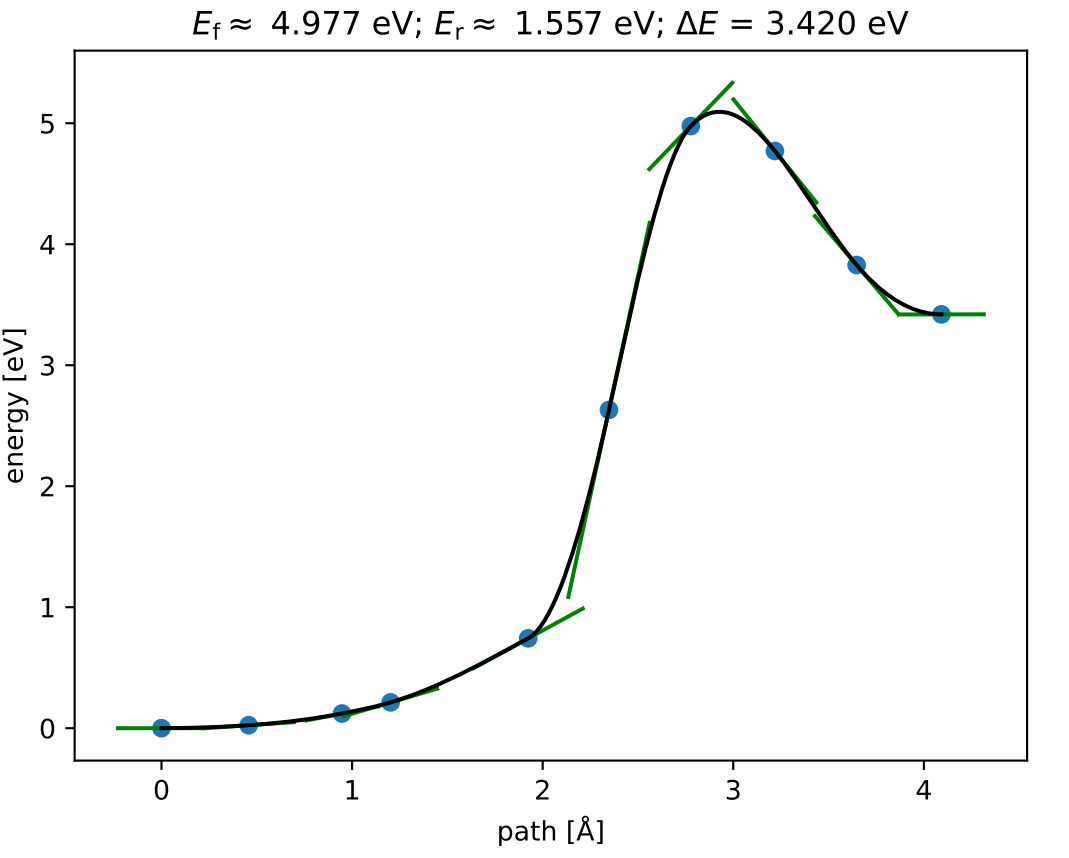
$E_f \approx$ 4.977 eV; $E_r \approx$ 1.557 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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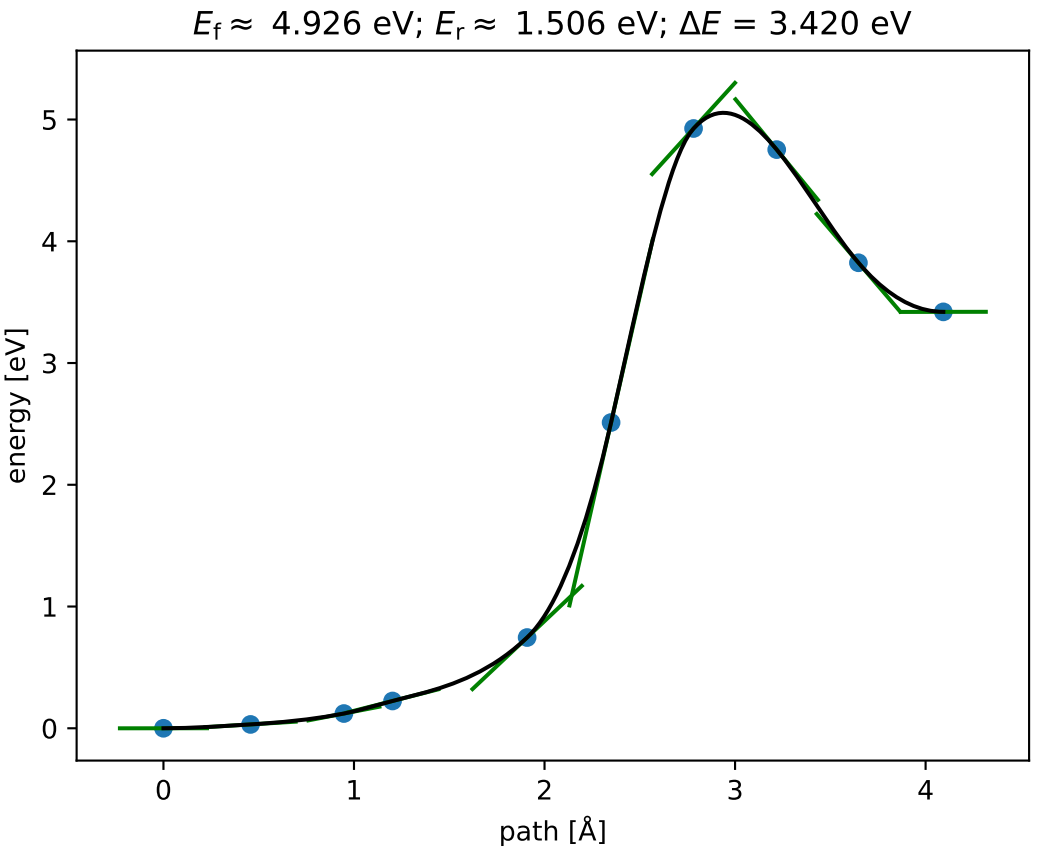
$E_f \approx$ 4.926 eV; $E_r \approx$ 1.506 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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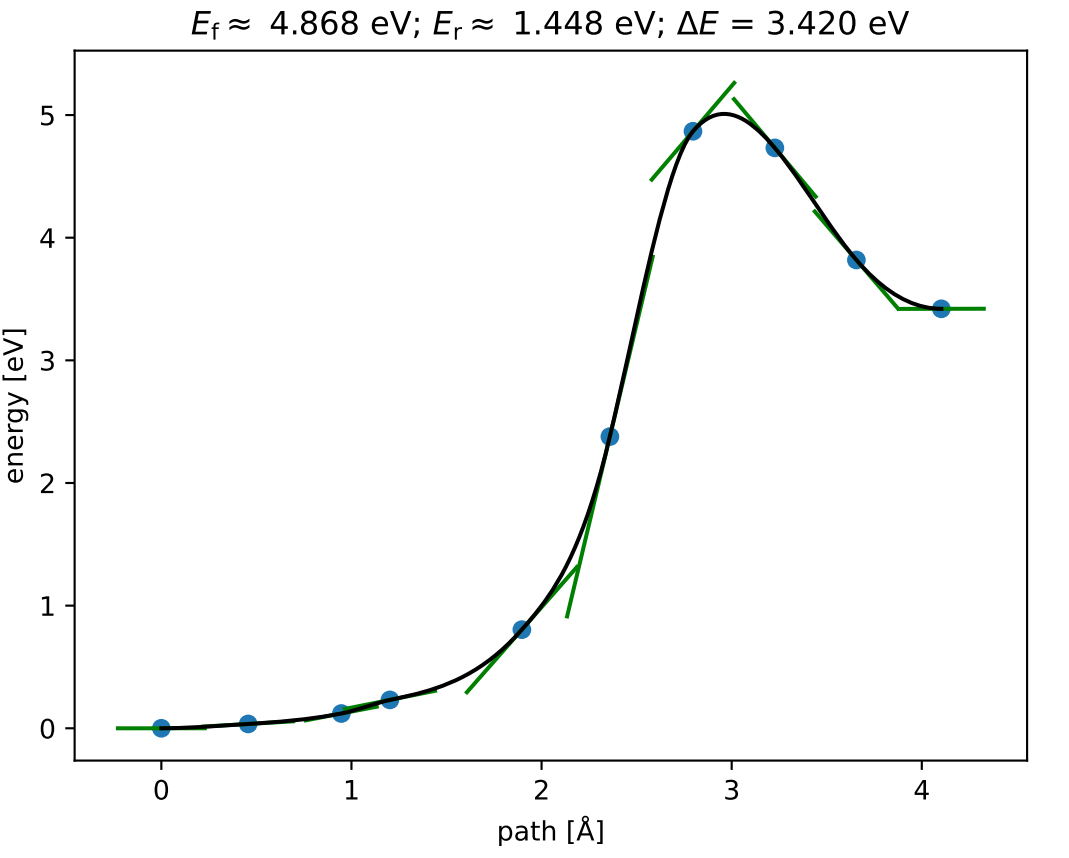
$E_f \approx$ 4.868 eV; $E_r \approx$ 1.448 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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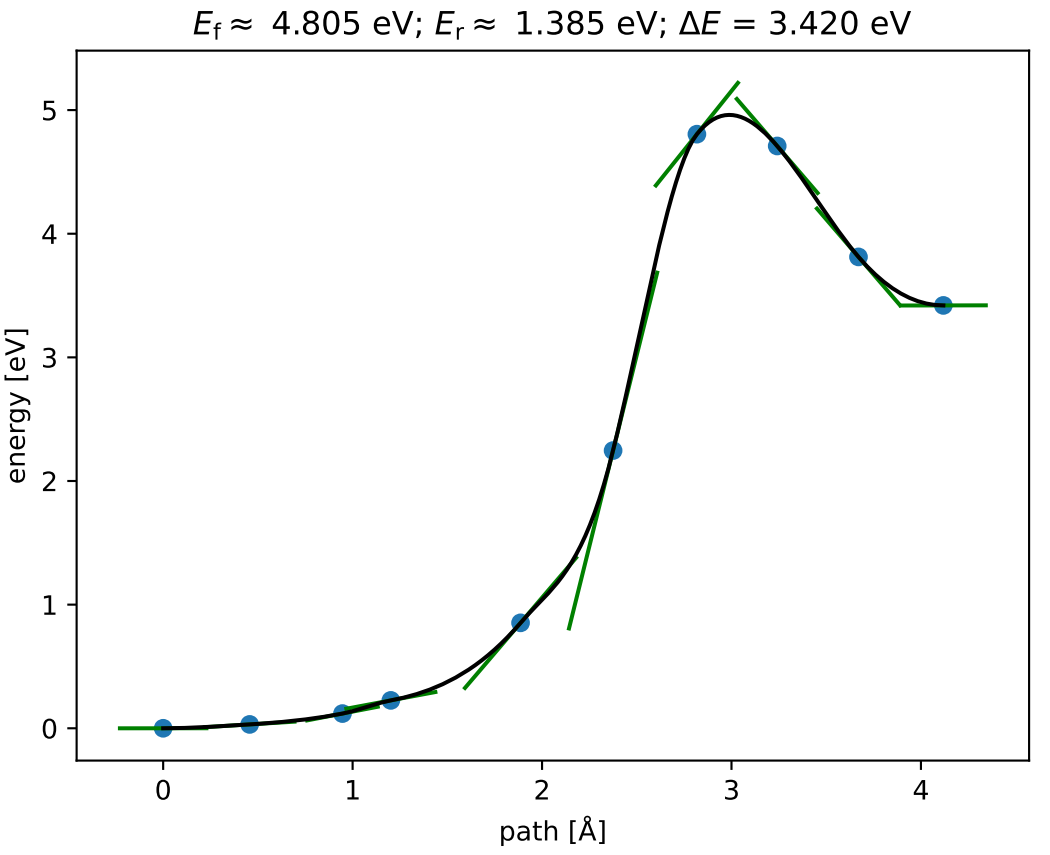
$E_f \approx$ 4.805 eV; $E_r \approx$ 1.385 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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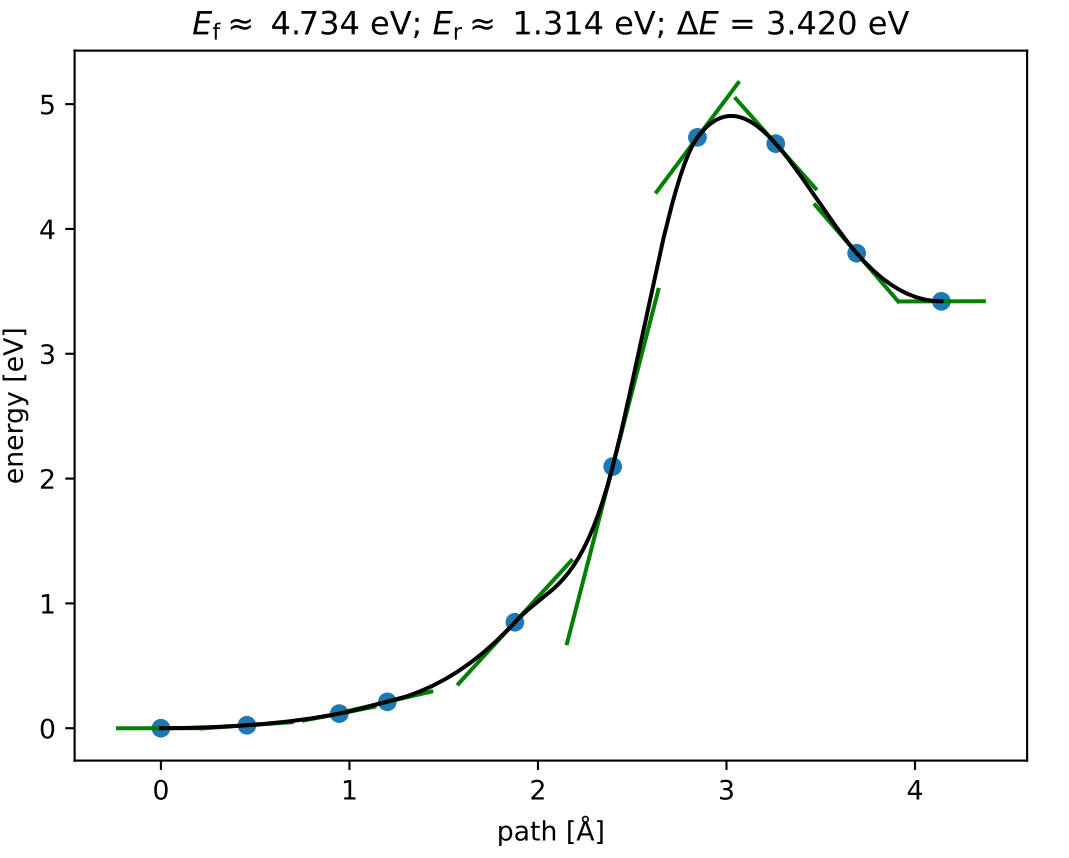
$E_f \approx$ 4.734 eV; $E_r \approx$ 1.314 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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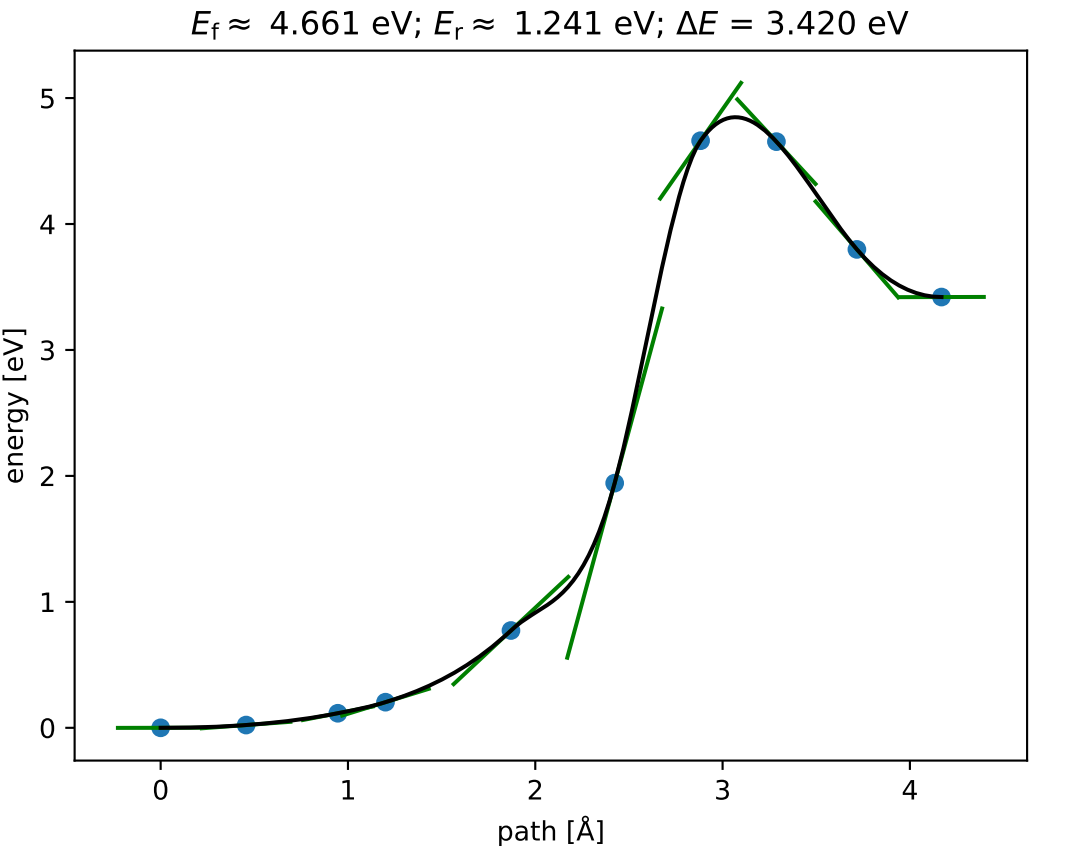
$E_f \approx$ 4.661 eV; $E_r \approx$ 1.241 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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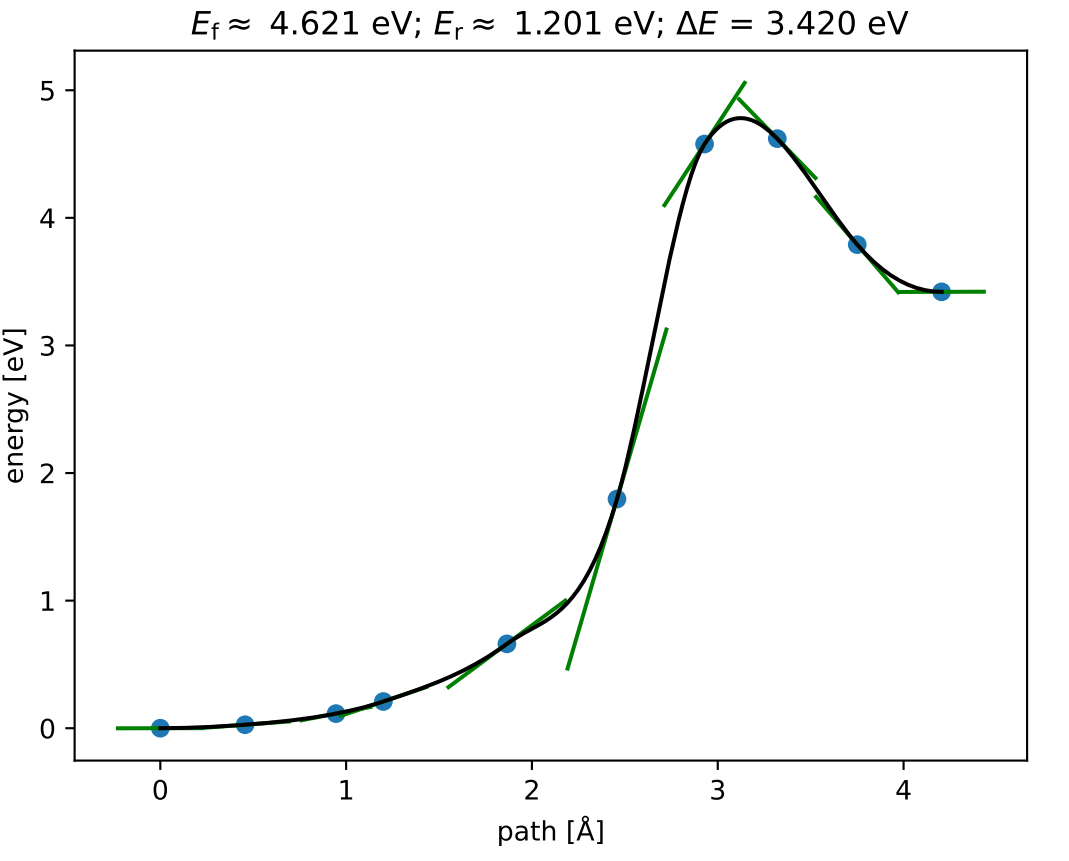
$E_f \approx$ 4.621 eV; $E_r \approx$ 1.201 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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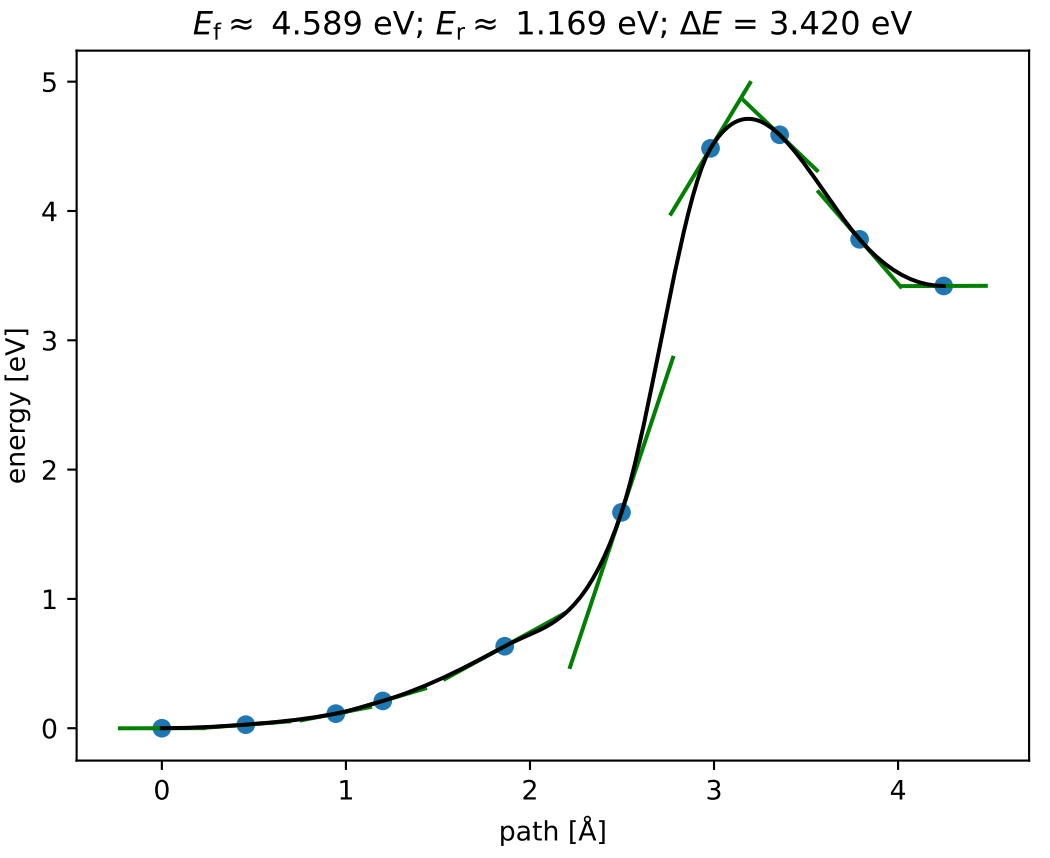
$E_f \approx$ 4.589 eV; $E_r \approx$ 1.169 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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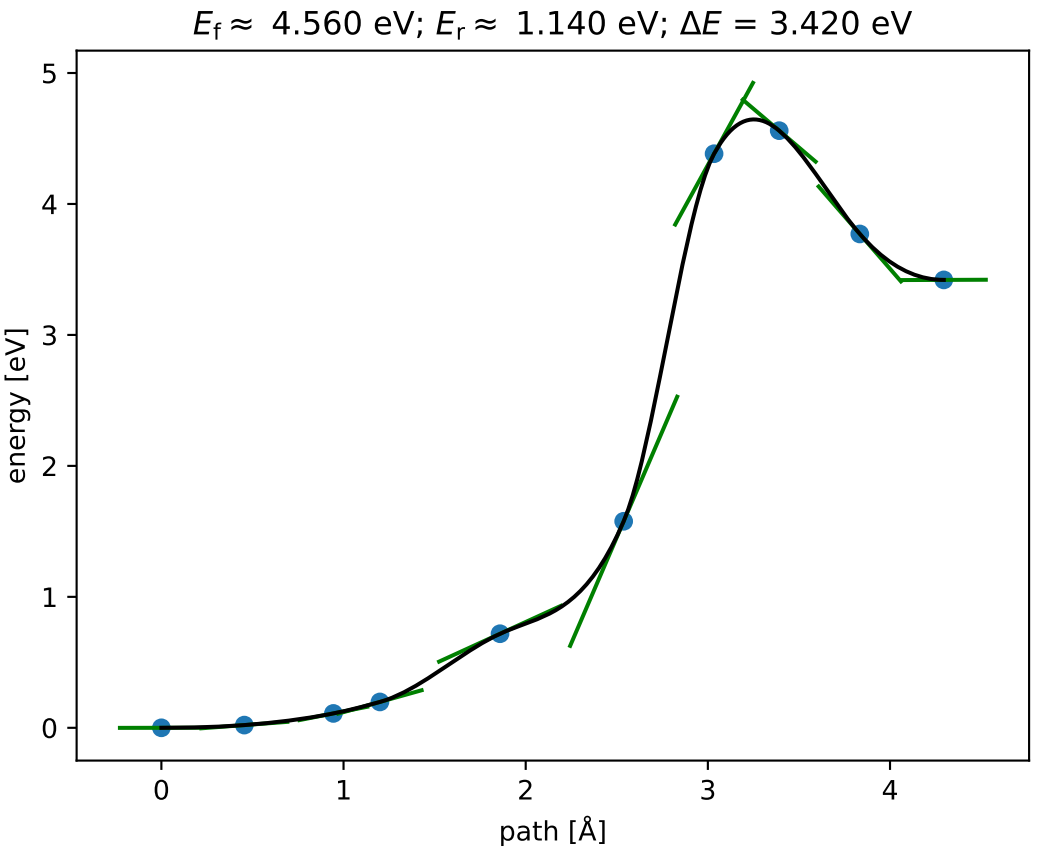
$E_f \approx$ 4.560 eV; $E_r \approx$ 1.140 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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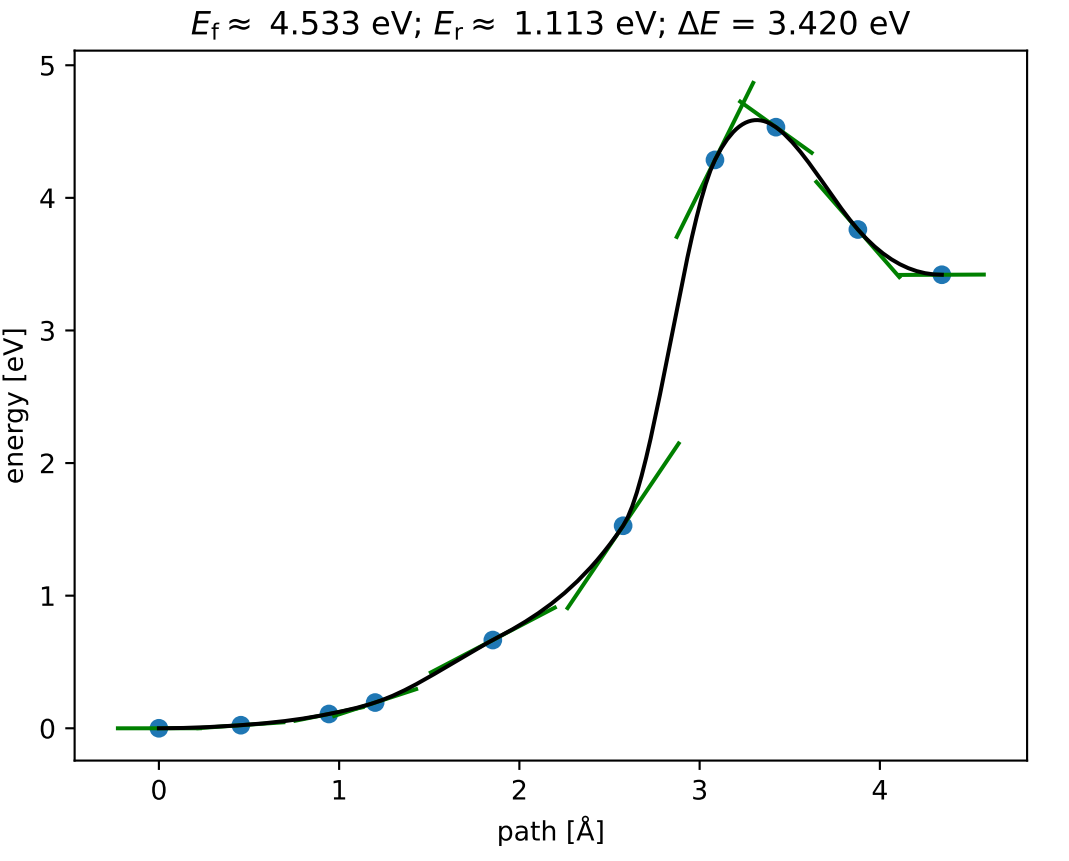
$E_f \approx$ 4.533 eV; $E_r \approx$ 1.113 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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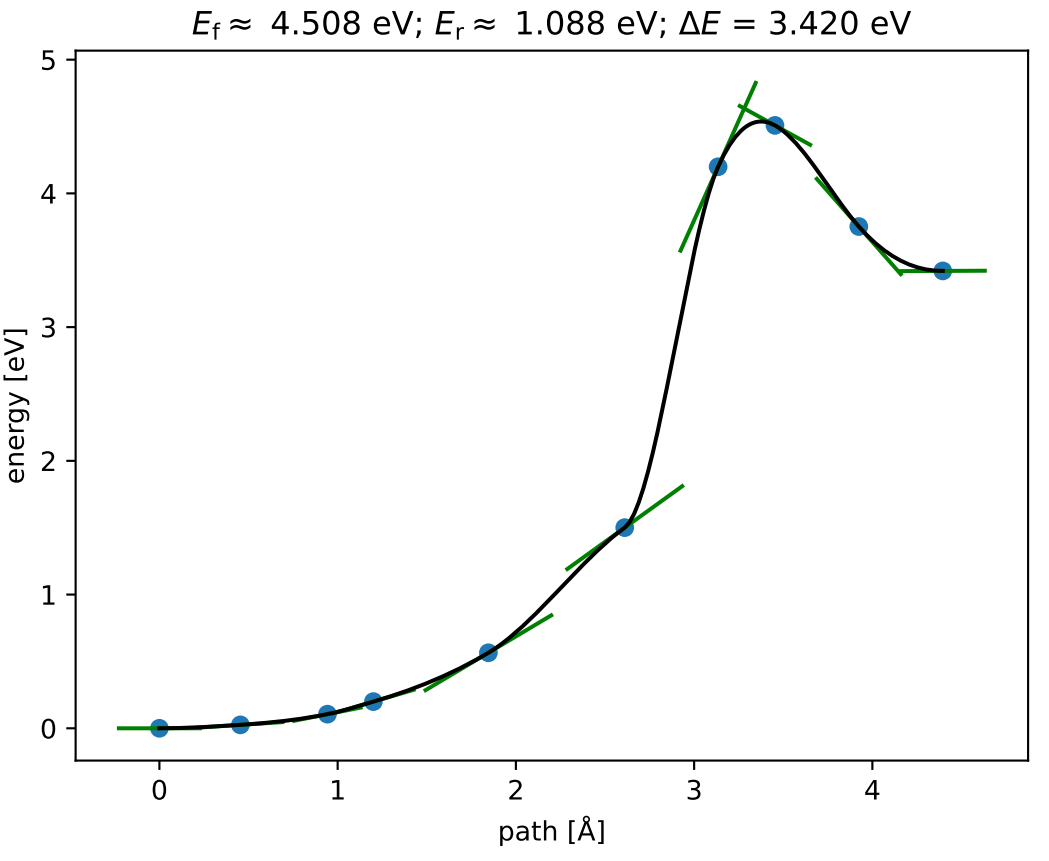
$E_f \approx$ 4.508 eV; $E_r \approx$ 1.088 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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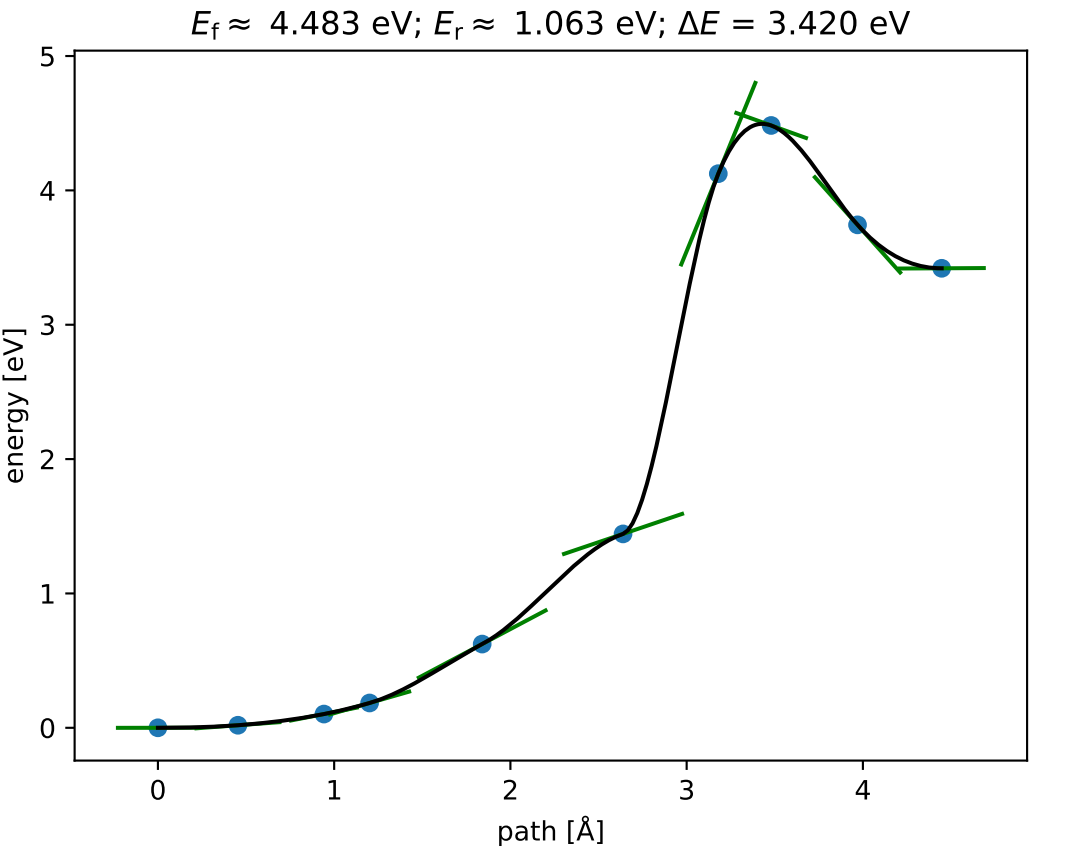
$E_f \approx$ 4.483 eV; $E_r \approx$ 1.063 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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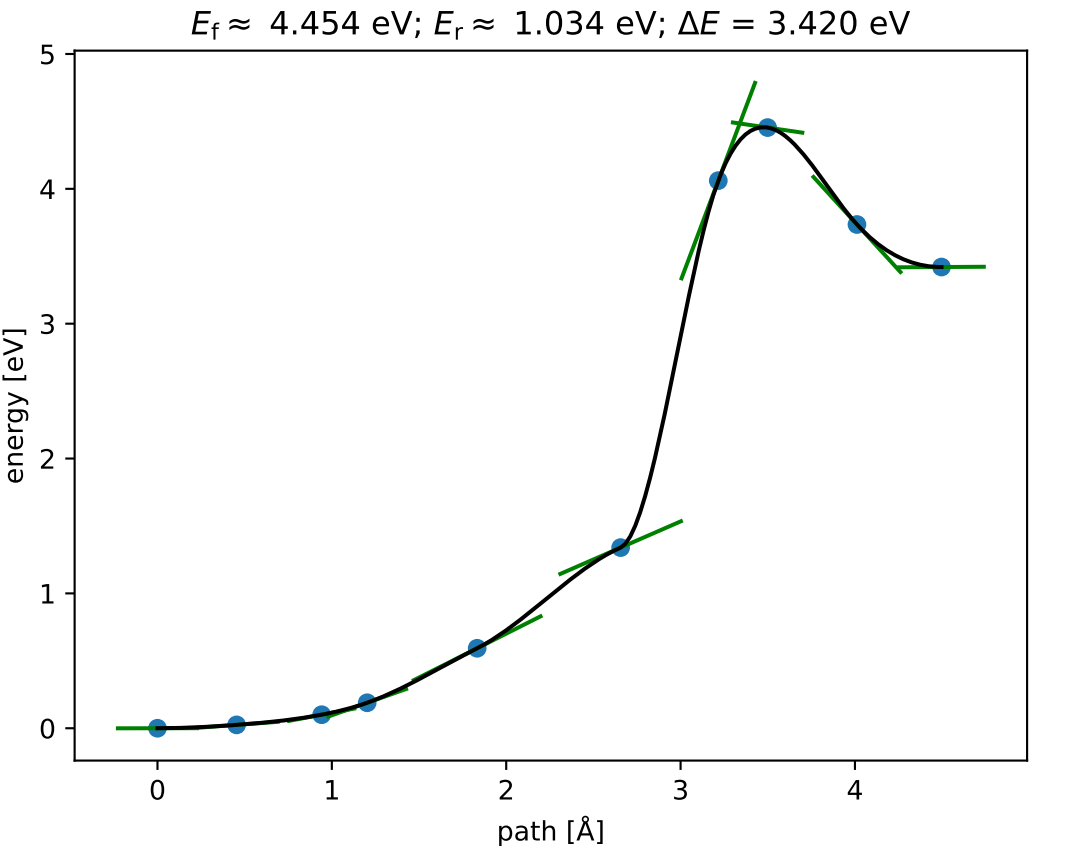
$E_f \approx$ 4.454 eV; $E_r \approx$ 1.034 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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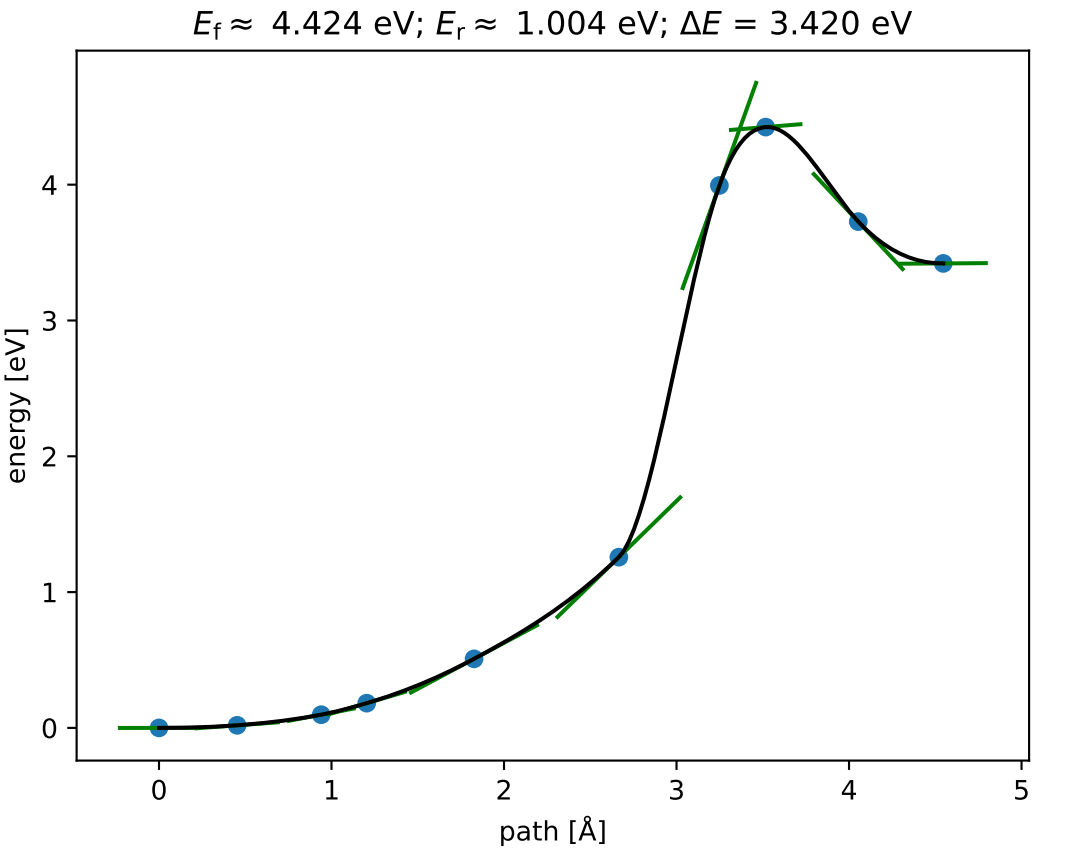
$E_f \approx$ 4.424 eV; $E_r \approx$ 1.004 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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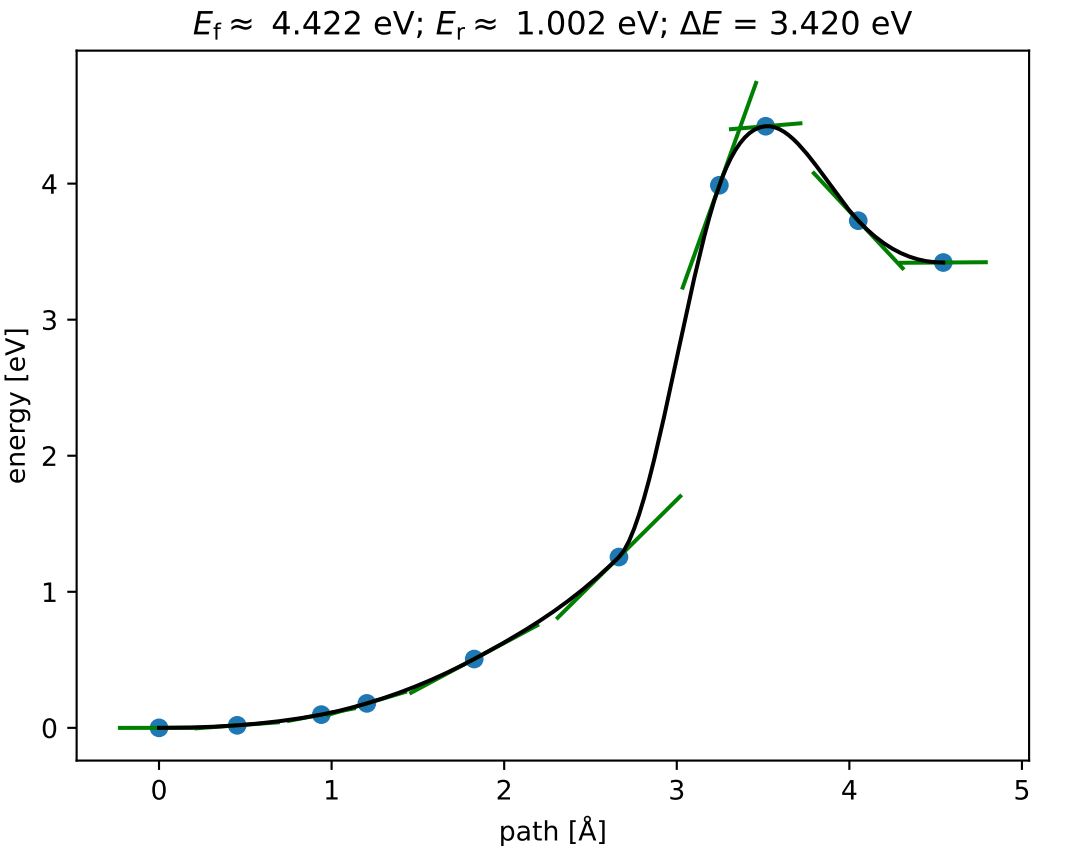
$E_f \approx$ 4.422 eV; $E_r \approx$ 1.002 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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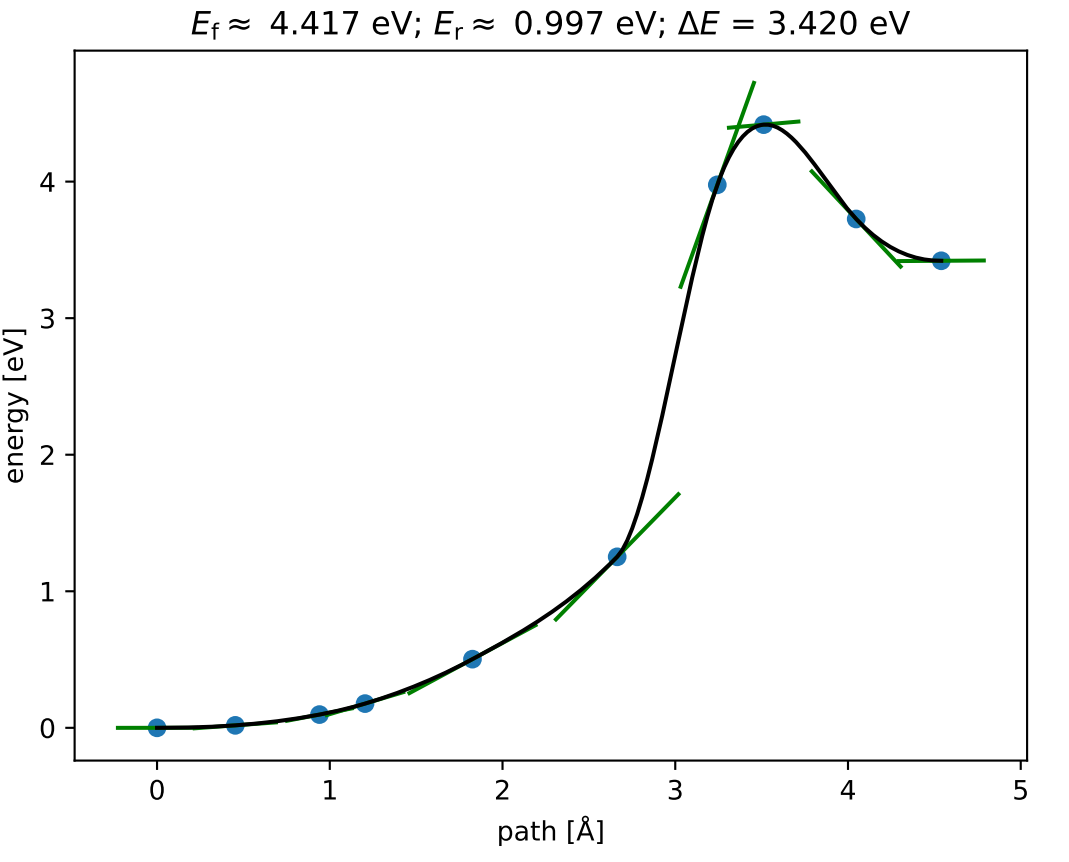
$E_f \approx$ 4.417 eV; $E_r \approx$ 0.997 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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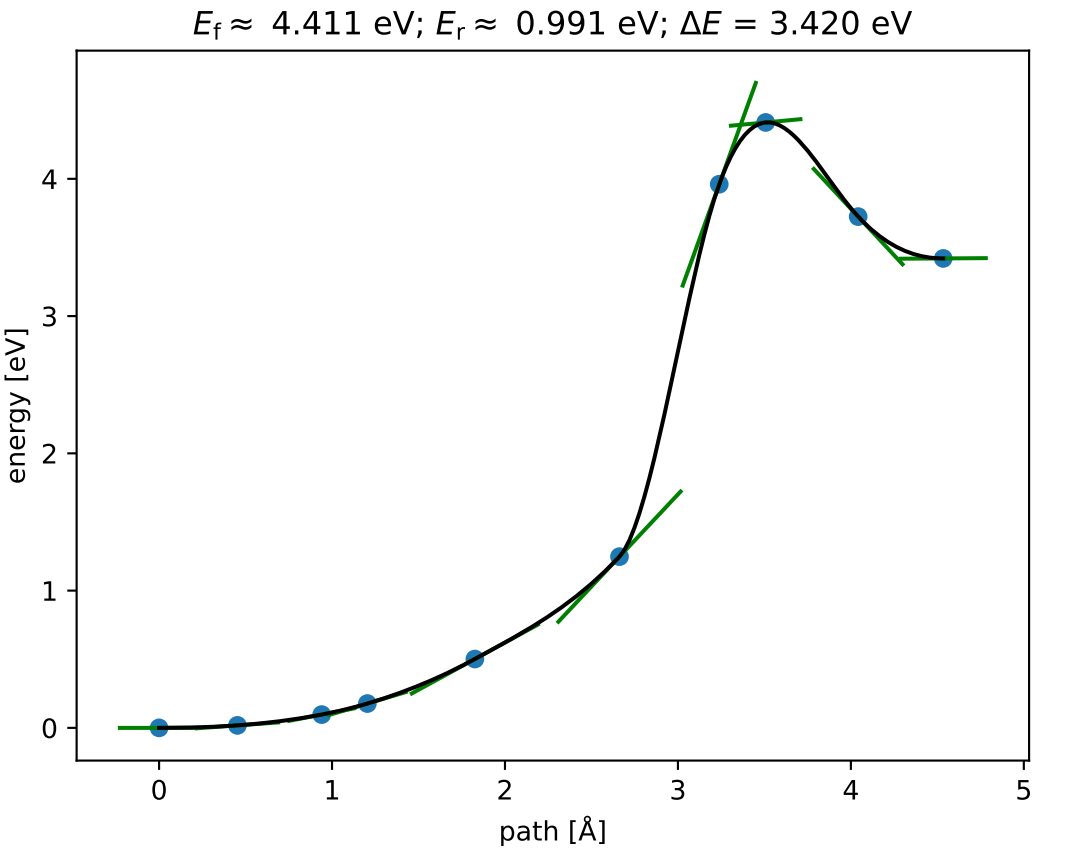
$E_f \approx$ 4.411 eV; $E_r \approx$ 0.991 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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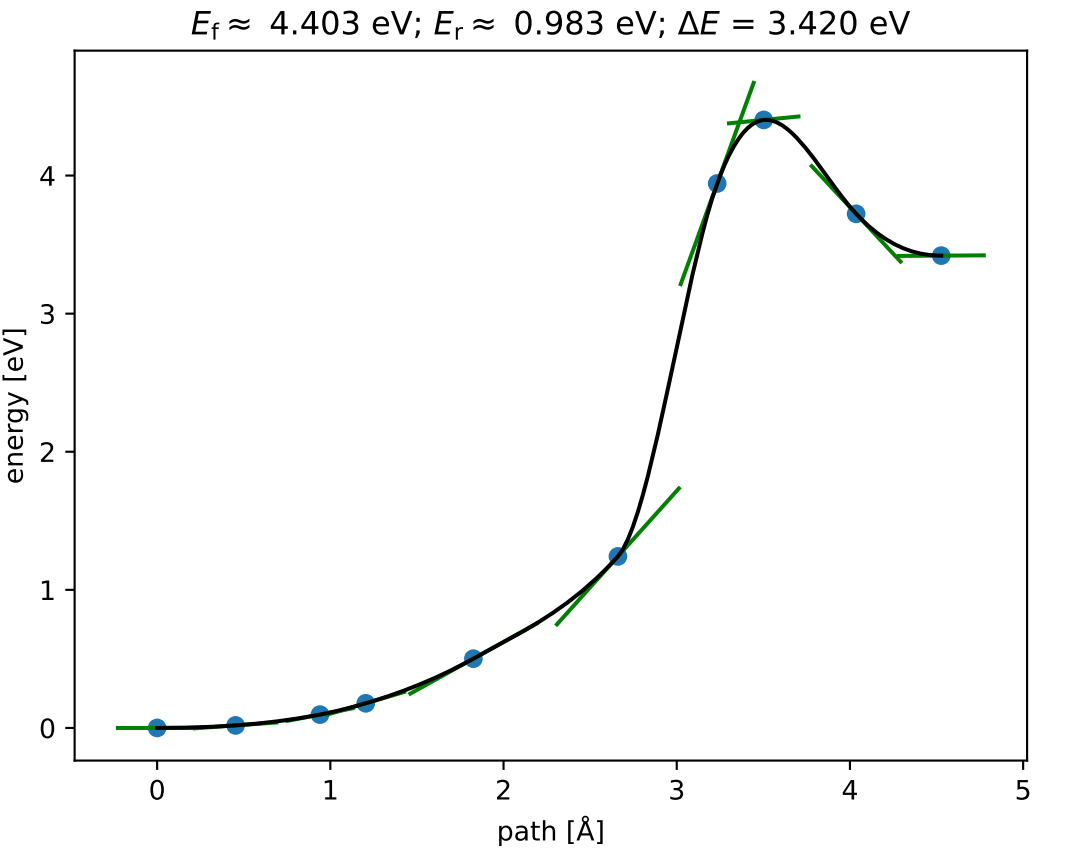
$E_f \approx$ 4.403 eV; $E_r \approx$ 0.983 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
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4
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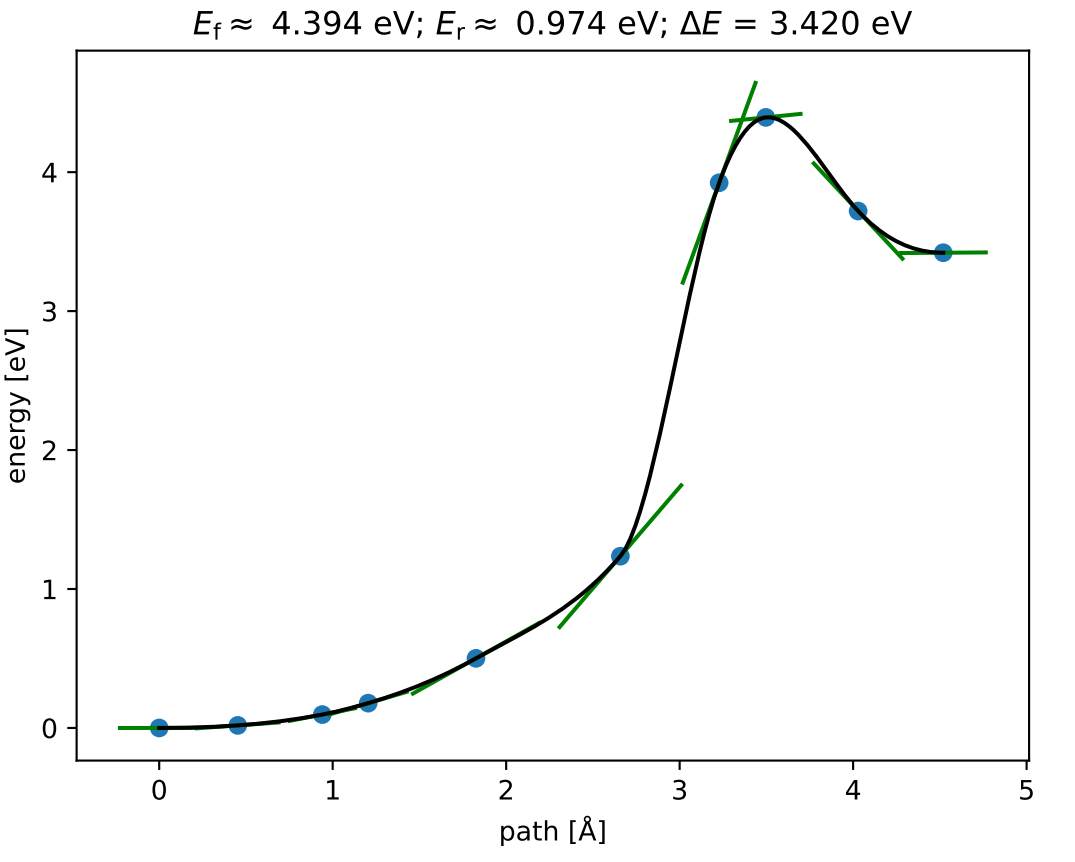
$E_f \approx$ 4.394 eV; $E_r \approx$ 0.974 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
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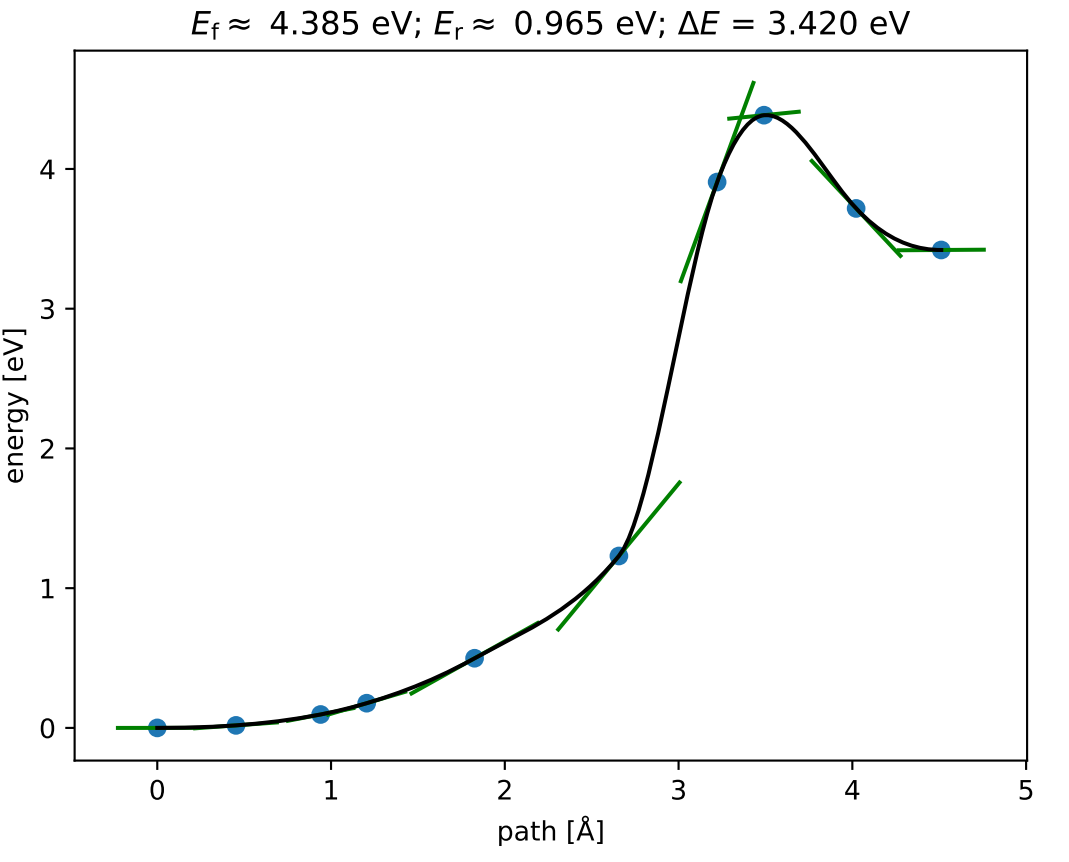
$E_f \approx$ 4.385 eV; $E_r \approx$ 0.965 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
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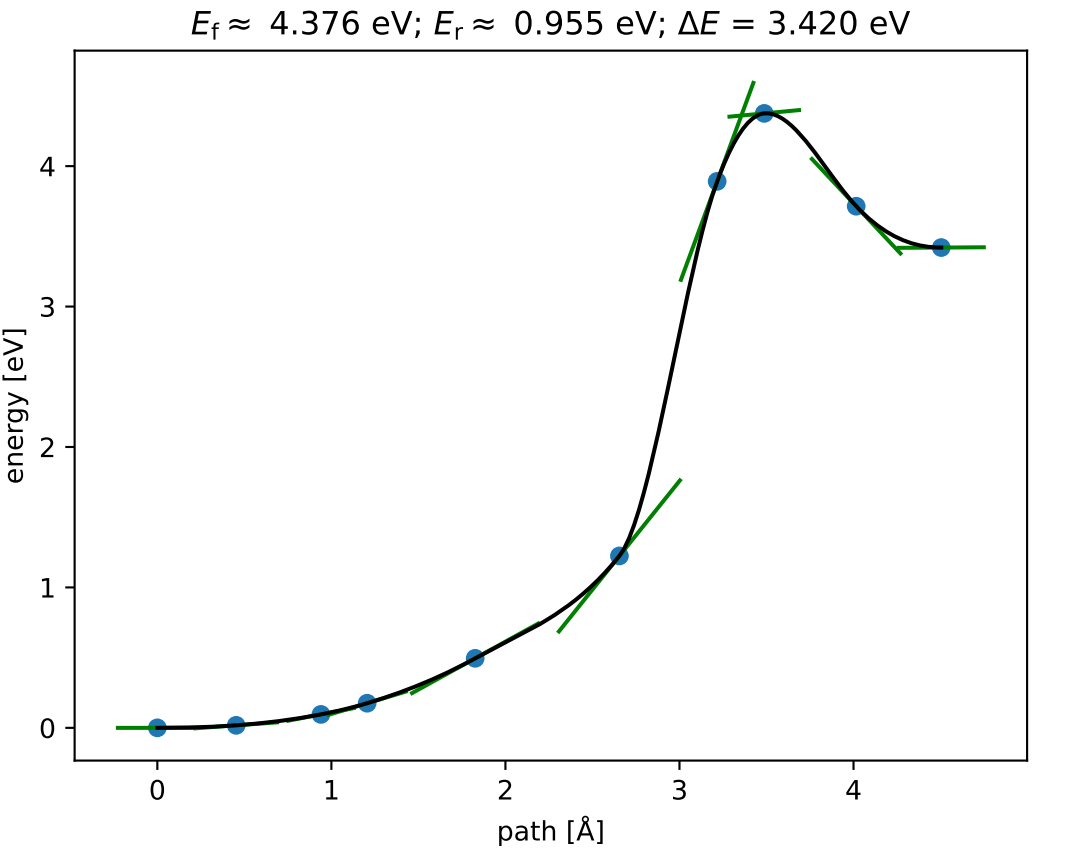
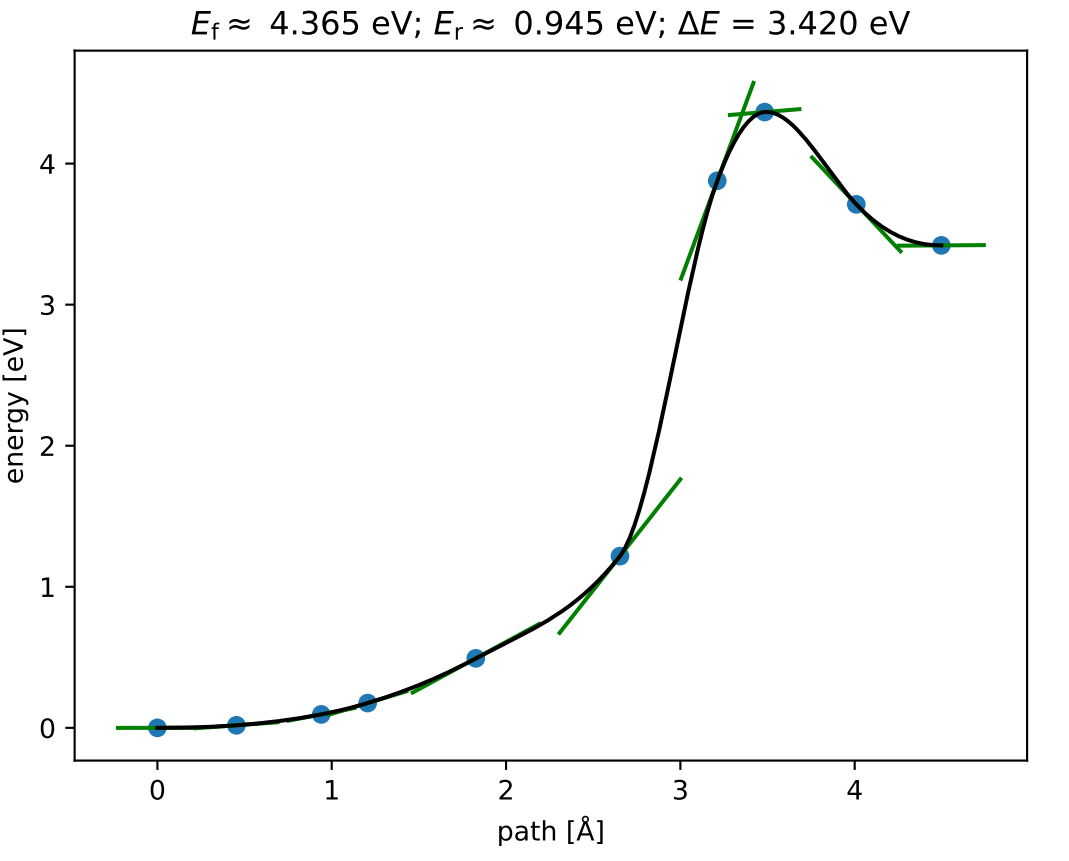
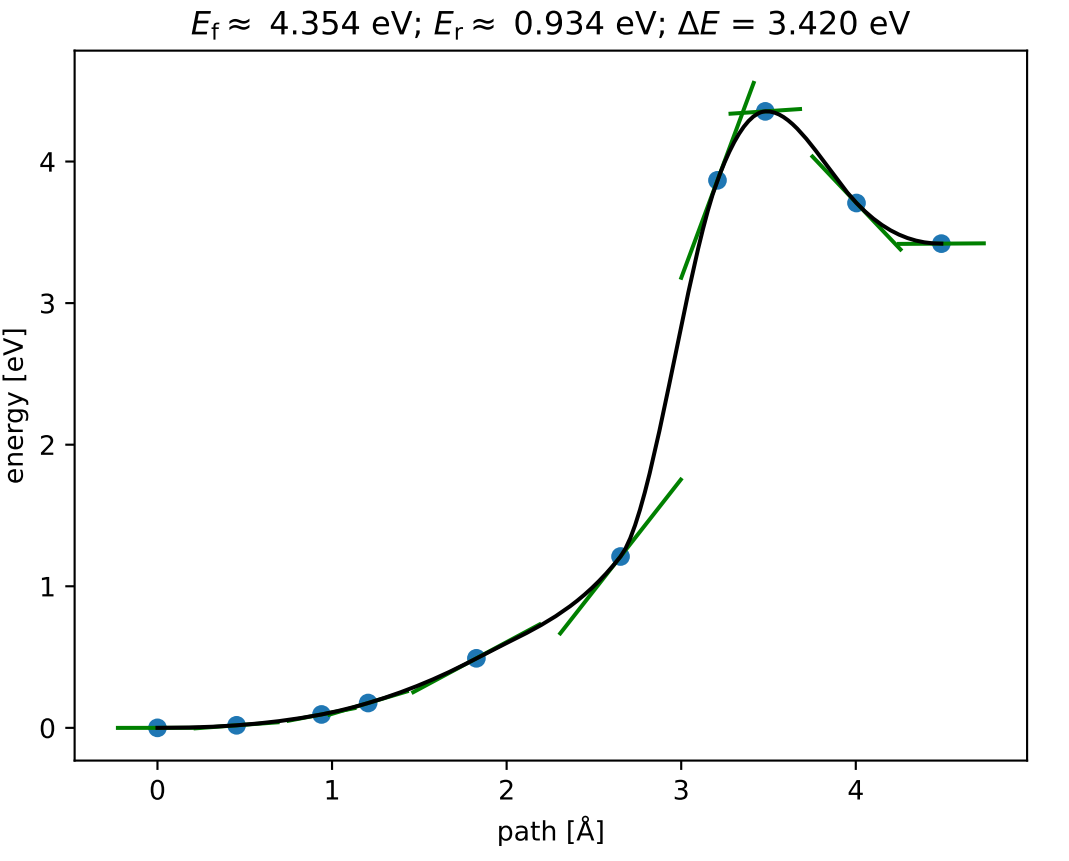
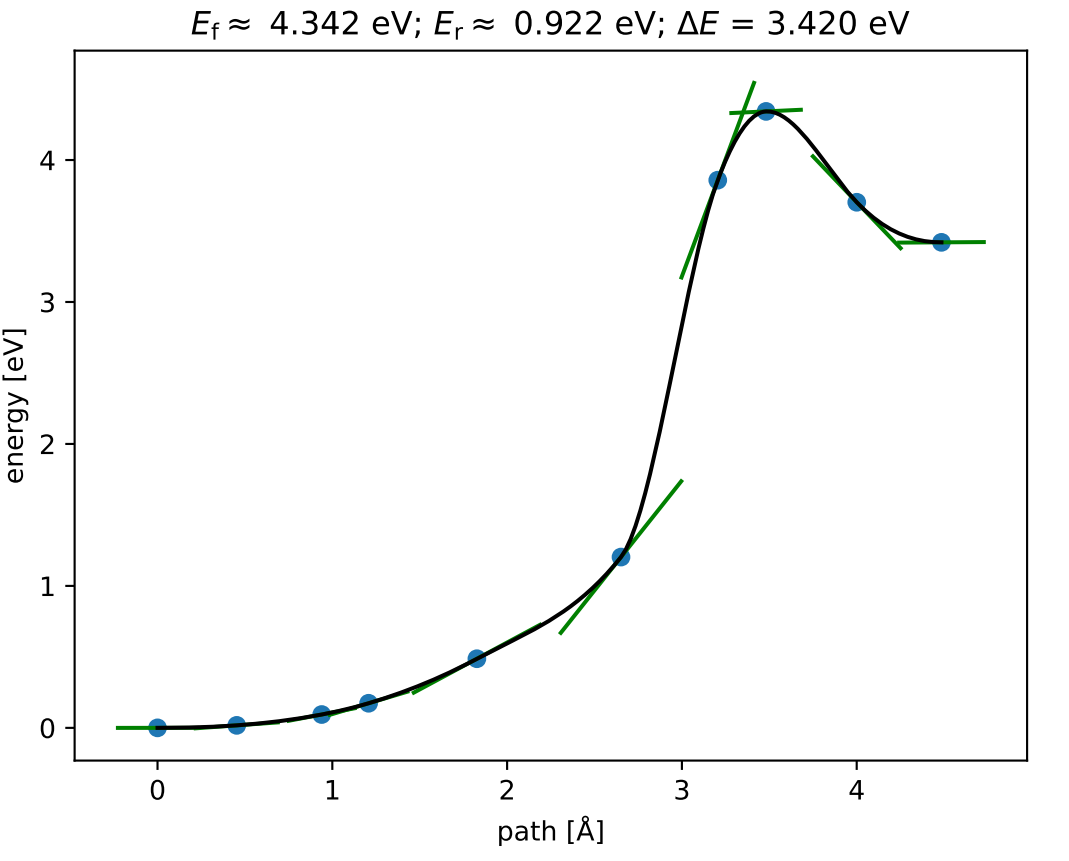
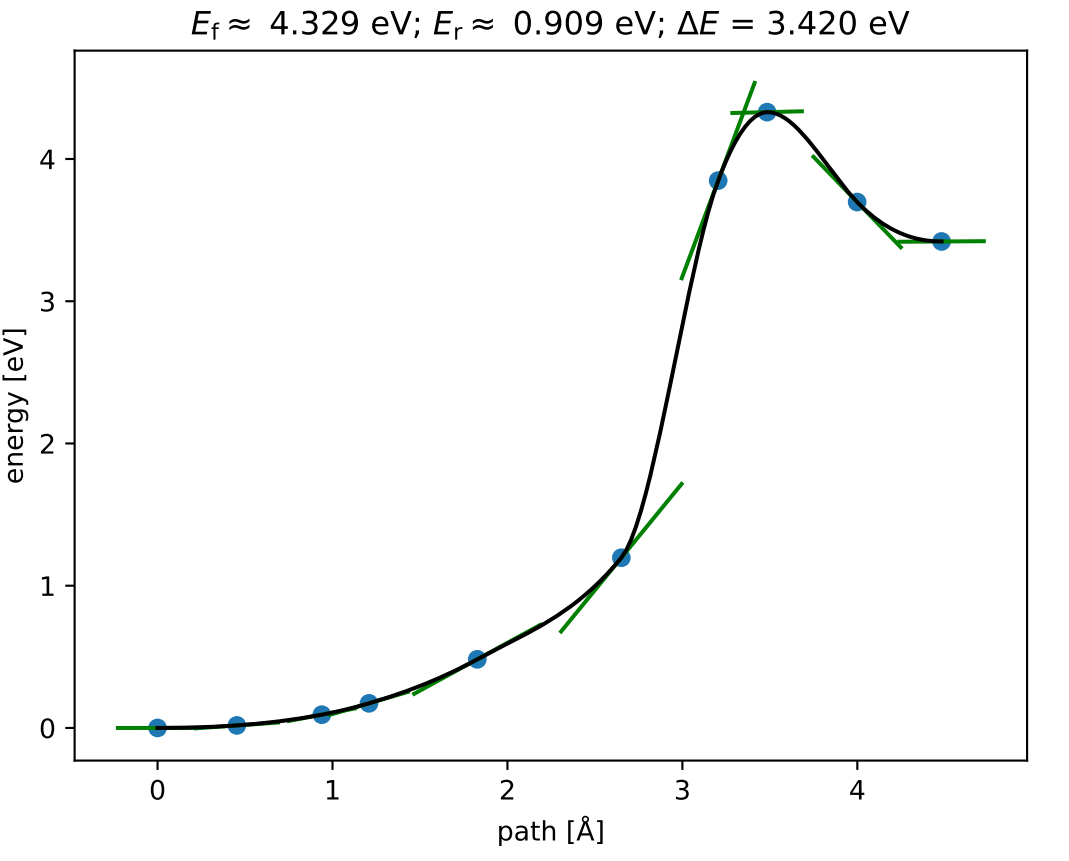
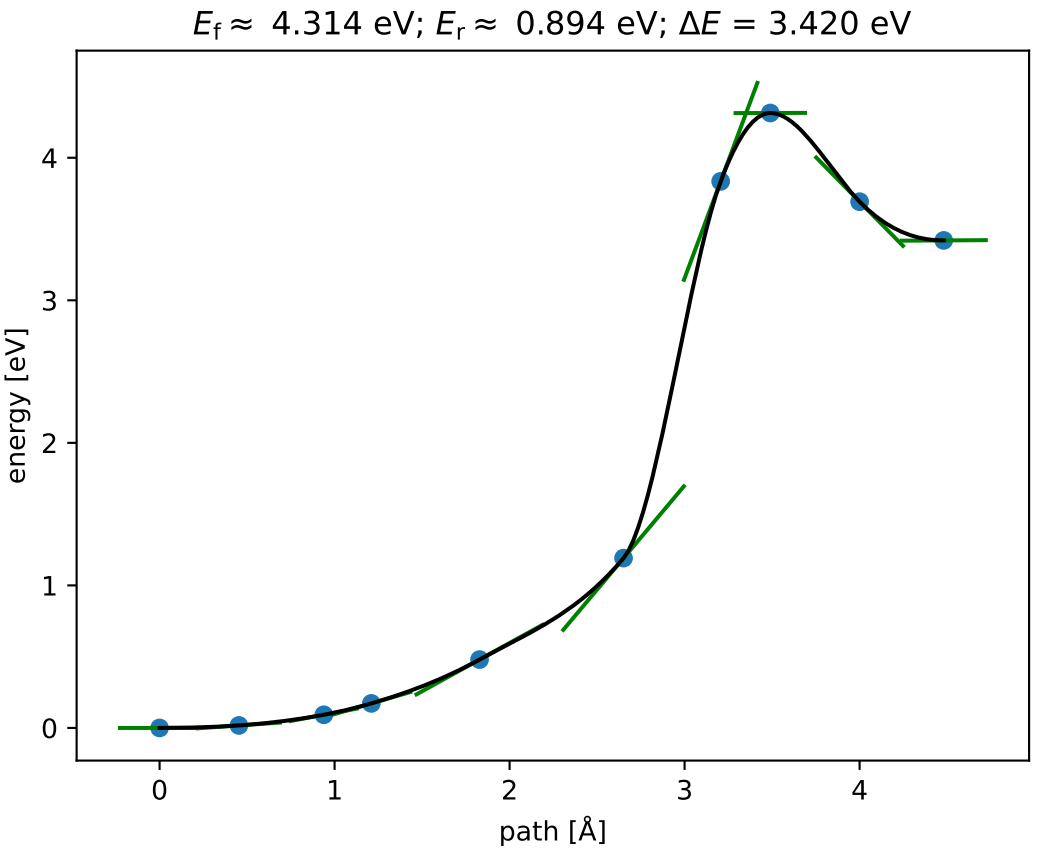

$E_f \approx$ 4.376 eV; $E_r \approx$ 0.955 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
2
3
4

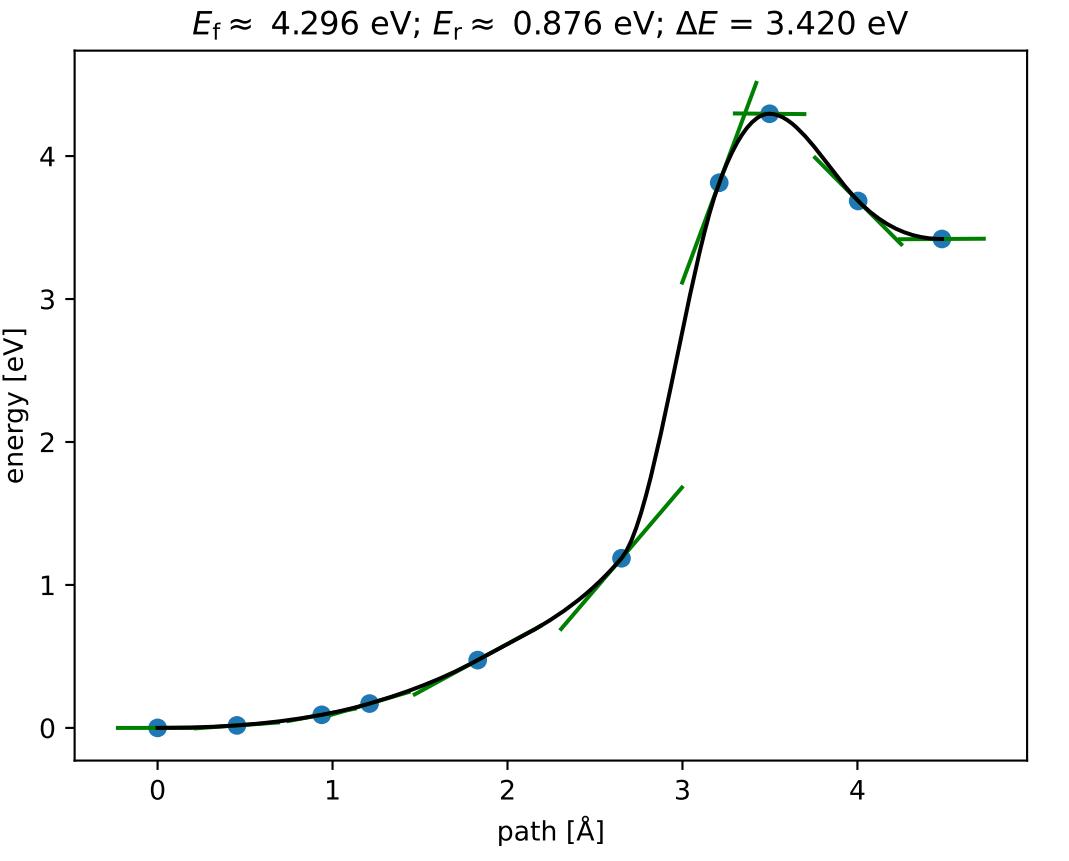

$E_f \approx$ 4.365 eV; $E_r \approx$ 0.945 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
2
3
4


$E_f \approx$ 4.354 eV; $E_r \approx$ 0.934 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
2
3
4


$E_f \approx$ 4.342 eV; $E_r \approx$ 0.922 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
2
3
4


$E_f \approx$ 4.329 eV; $E_r \approx$ 0.909 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
2
3
4


$E_f \approx$ 4.314 eV; $E_r \approx$ 0.894 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
2
3
4


$E_f \approx$ 4.296 eV; $E_r \approx$ 0.876 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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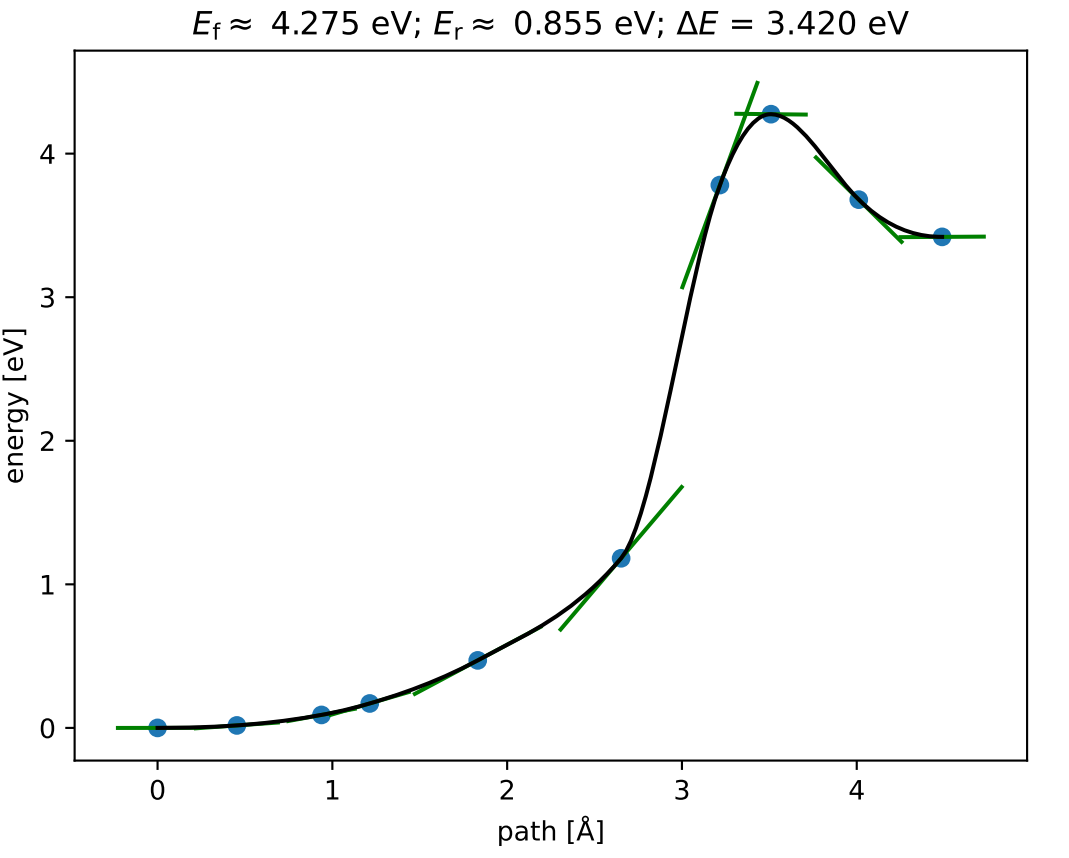
$E_f \approx$ 4.275 eV; $E_r \approx$ 0.855 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
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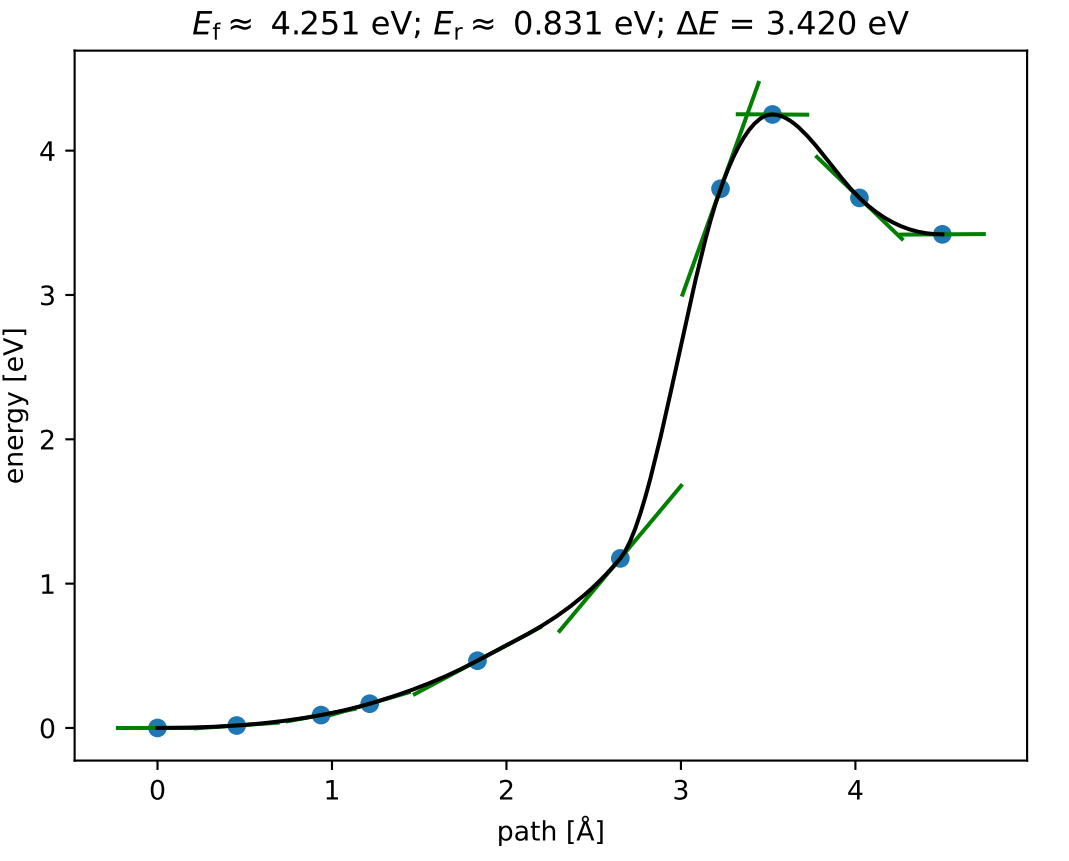
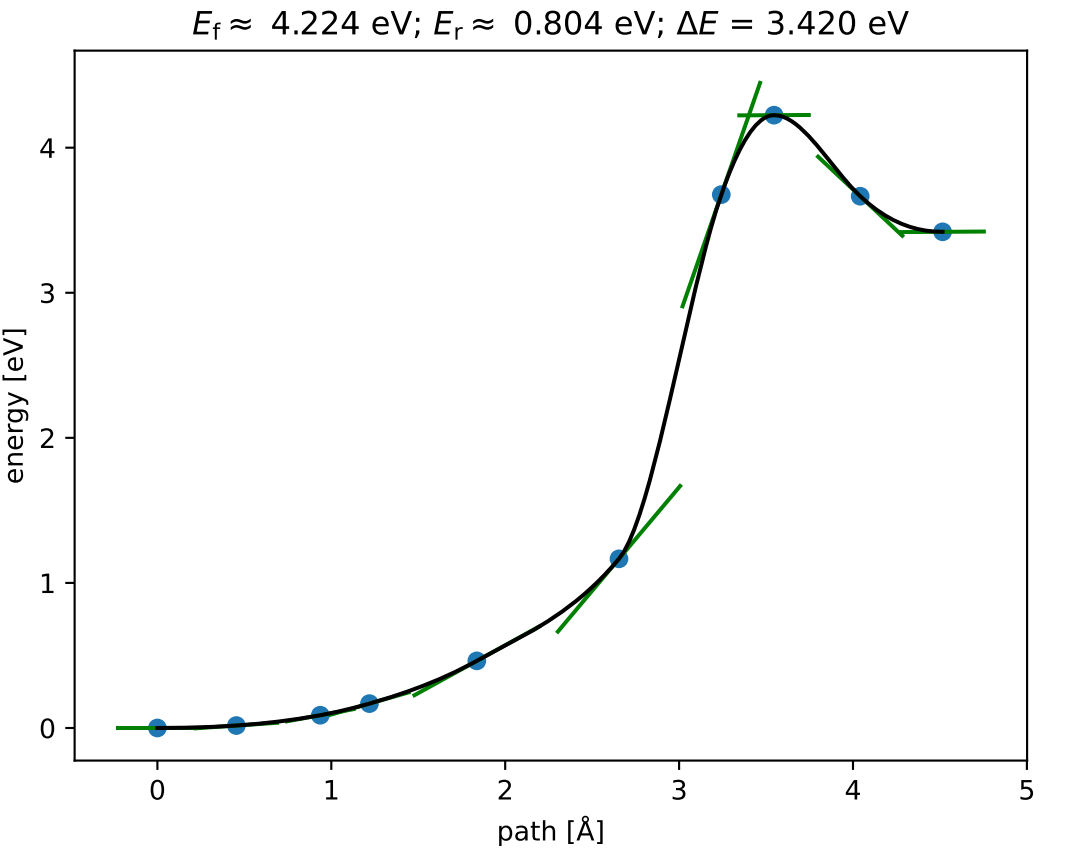
4


$E_f \approx$ 4.251 eV; $E_r \approx$ 0.831 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
2
3
4


$E_f \approx$ 4.224 eV; $E_r \approx$ 0.804 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
2
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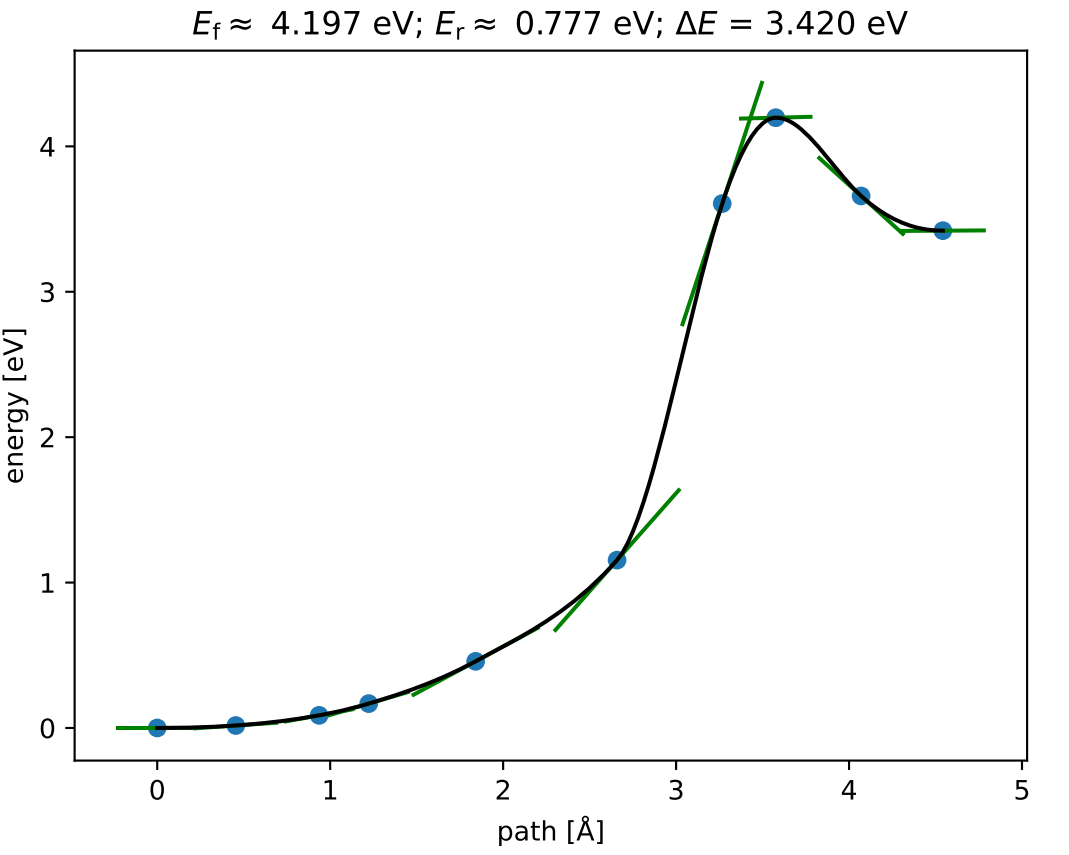
4
5


$E_f \approx$ 4.197 eV; $E_r \approx$ 0.777 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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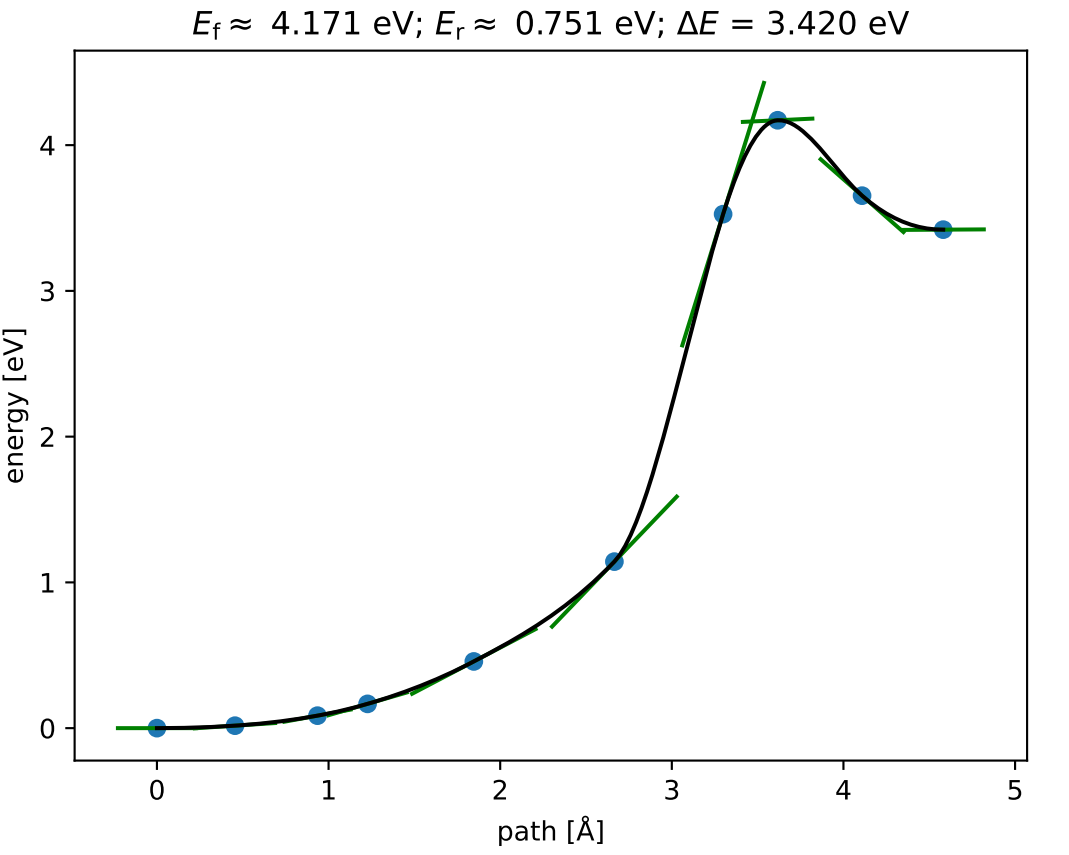
4
5


$E_f \approx$ 4.171 eV; $E_r \approx$ 0.751 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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4
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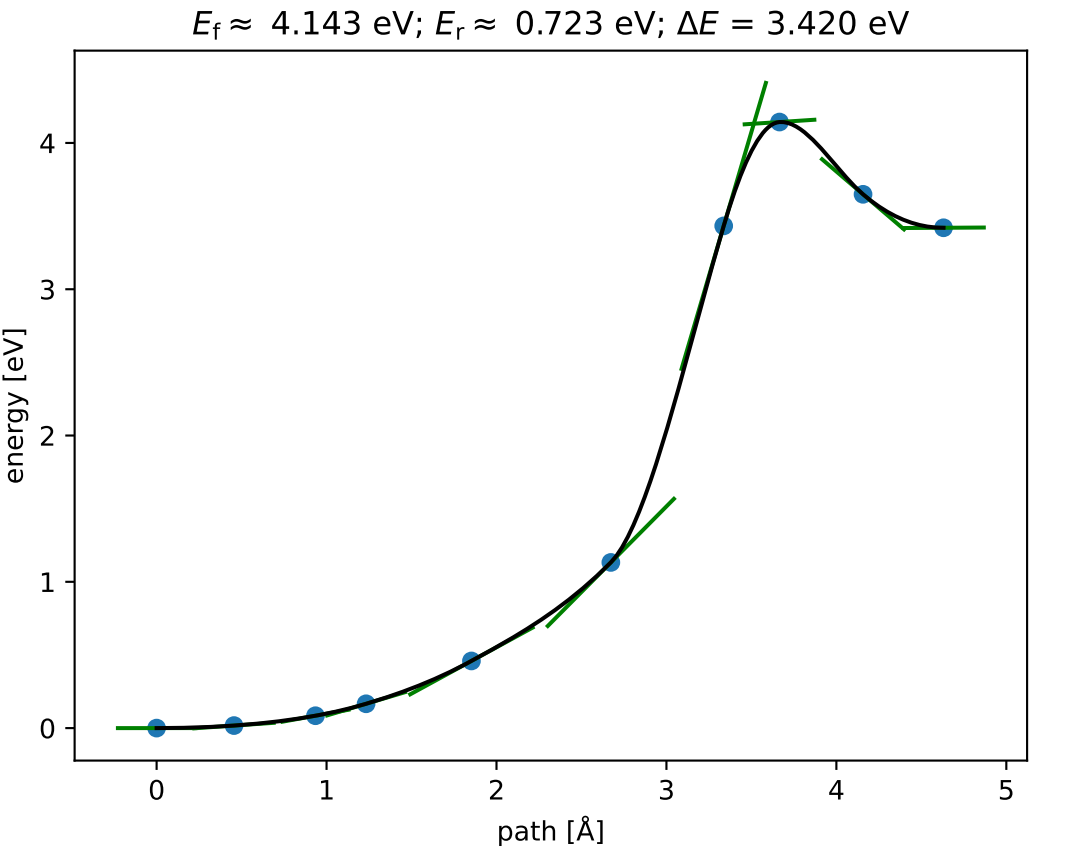
$E_f \approx$ 4.143 eV; $E_r \approx$ 0.723 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
2
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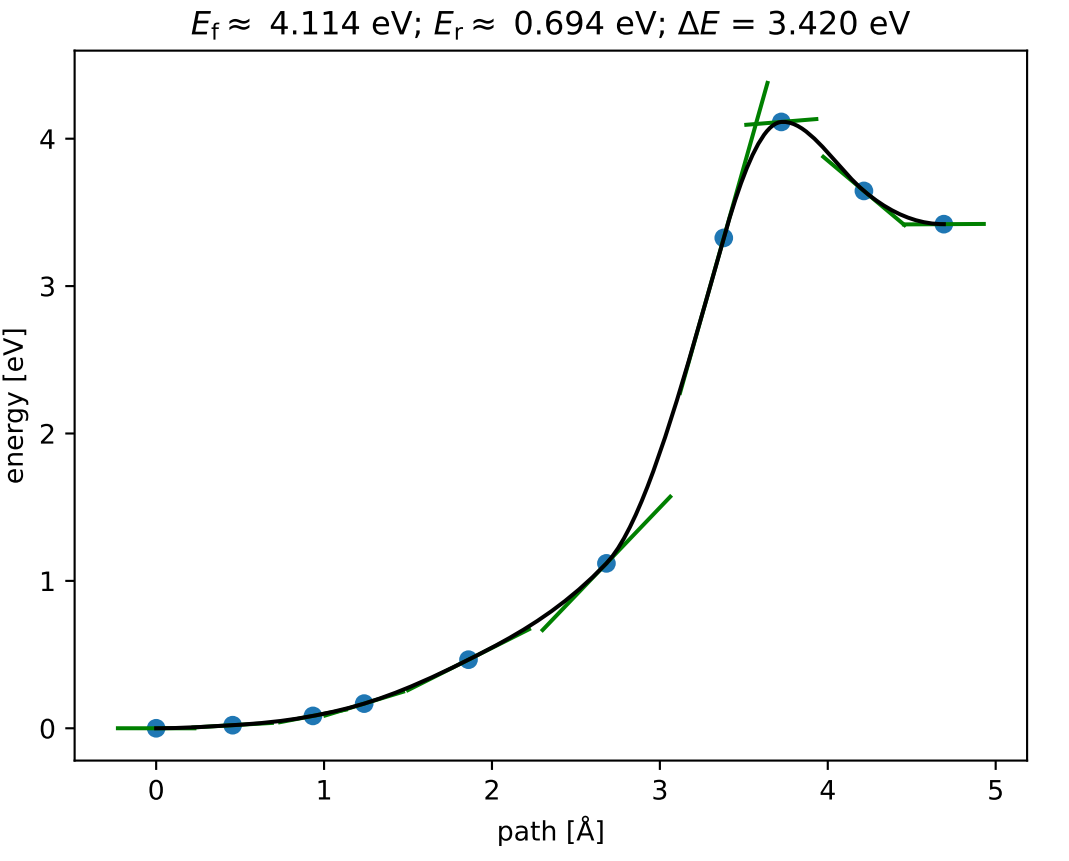
4
5


$E_f \approx$ 4.114 eV; $E_r \approx$ 0.694 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
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4
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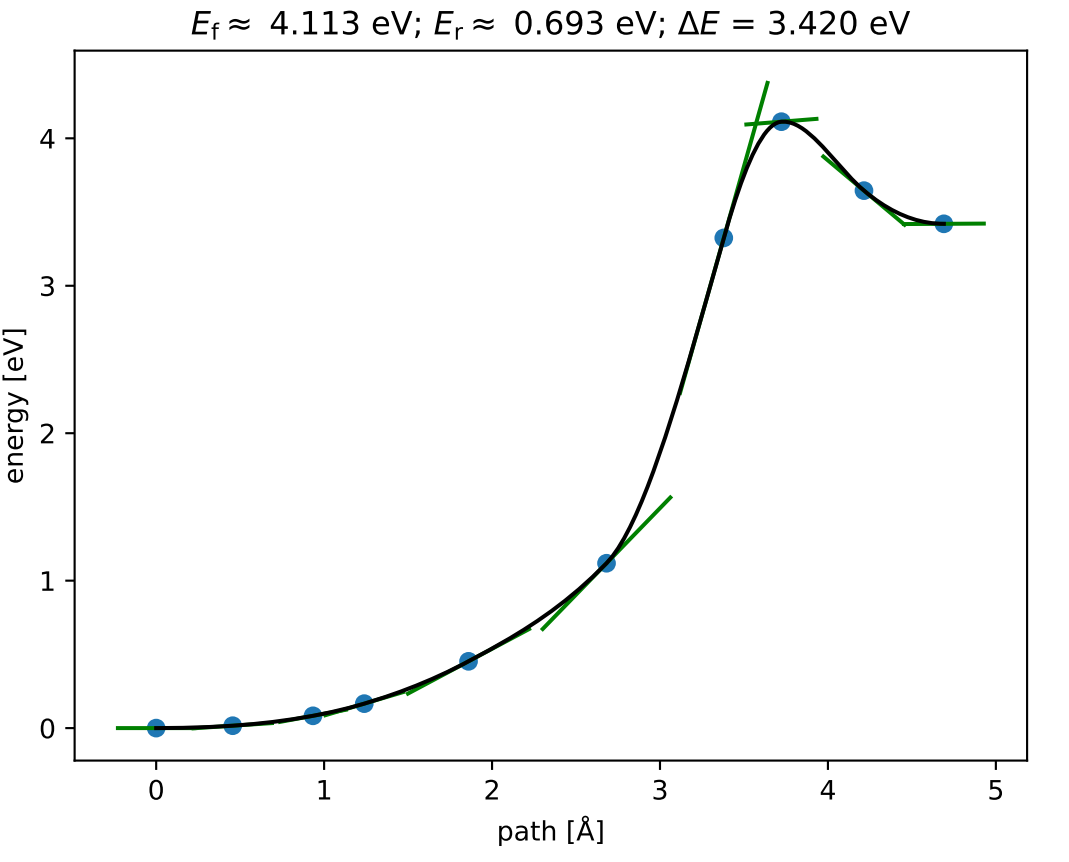
$E_f \approx$ 4.113 eV; $E_r \approx$ 0.693 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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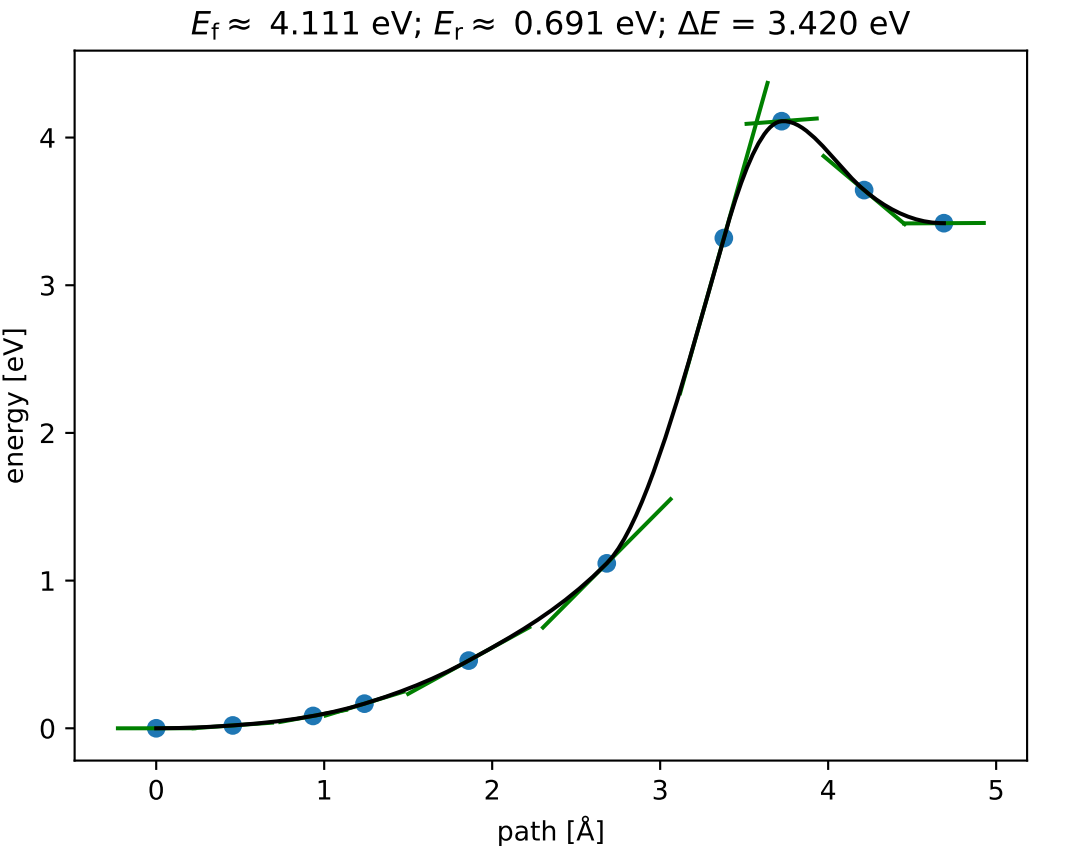
$E_f \approx$ 4.111 eV; $E_r \approx$ 0.691 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
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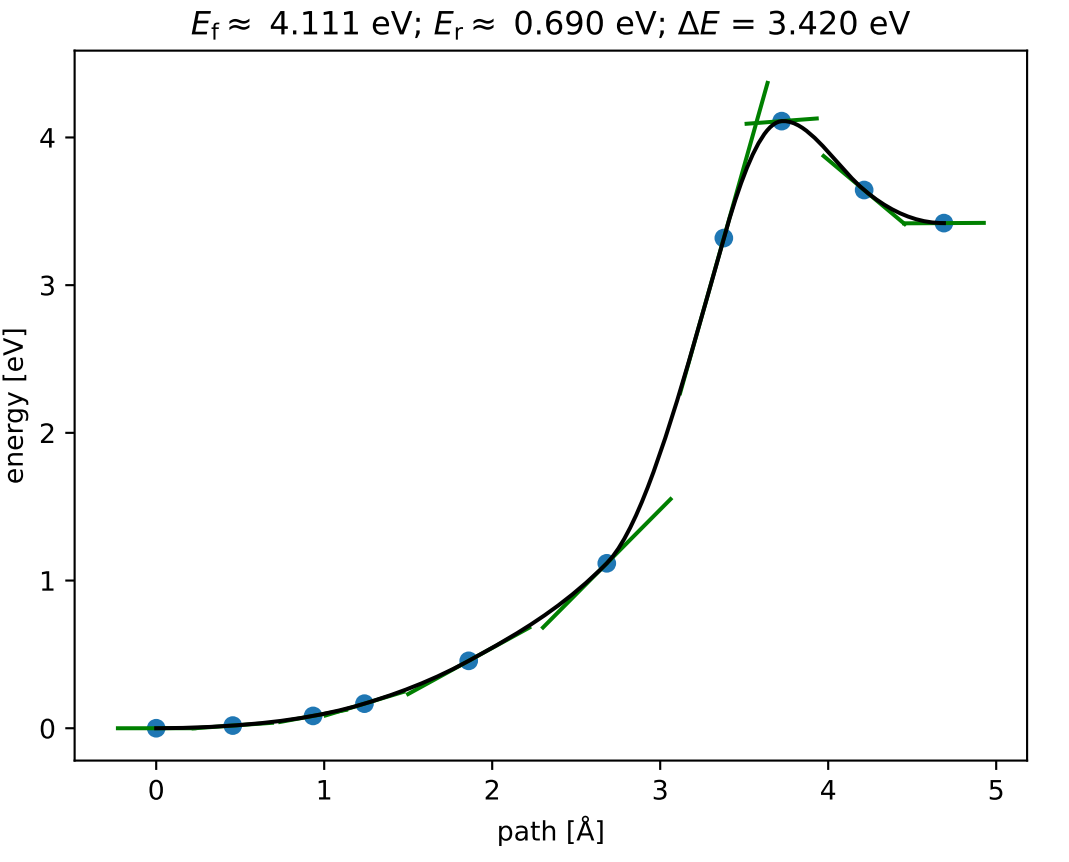
3
4
5


$E_f \approx$ 4.111 eV; $E_r \approx$ 0.690 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
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4
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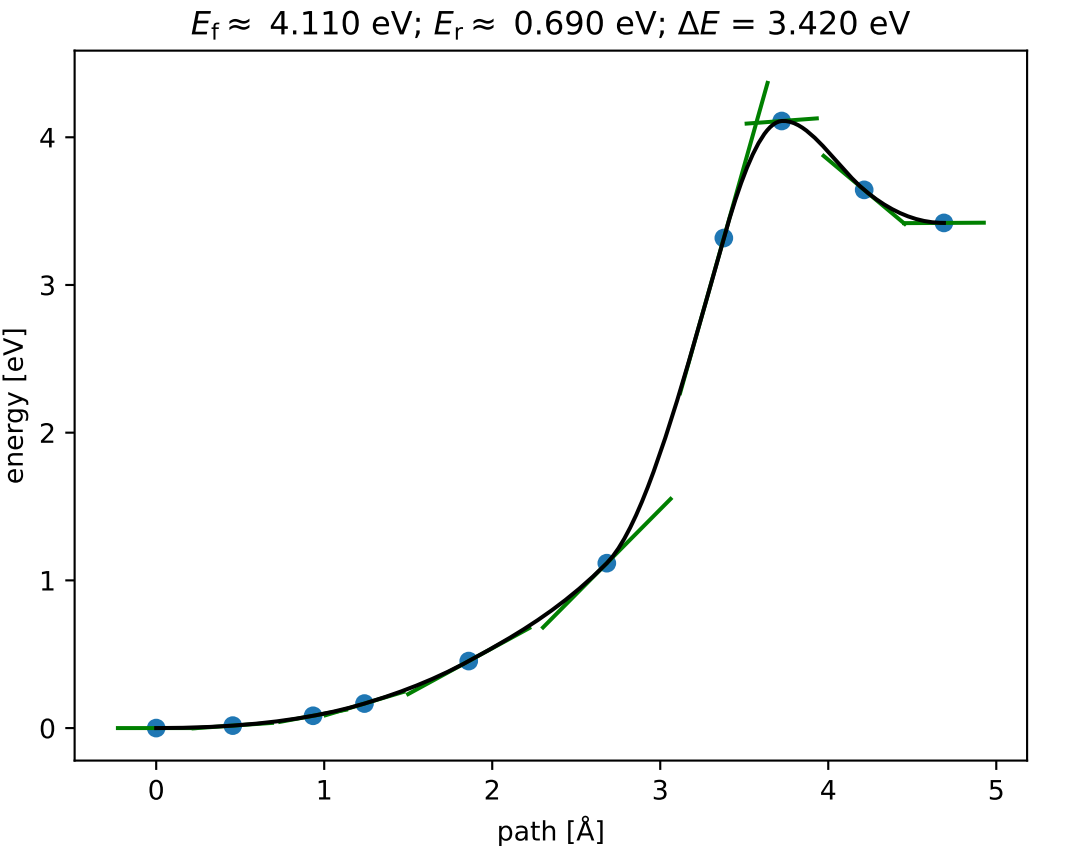
$E_f \approx$ 4.110 eV; $E_r \approx$ 0.690 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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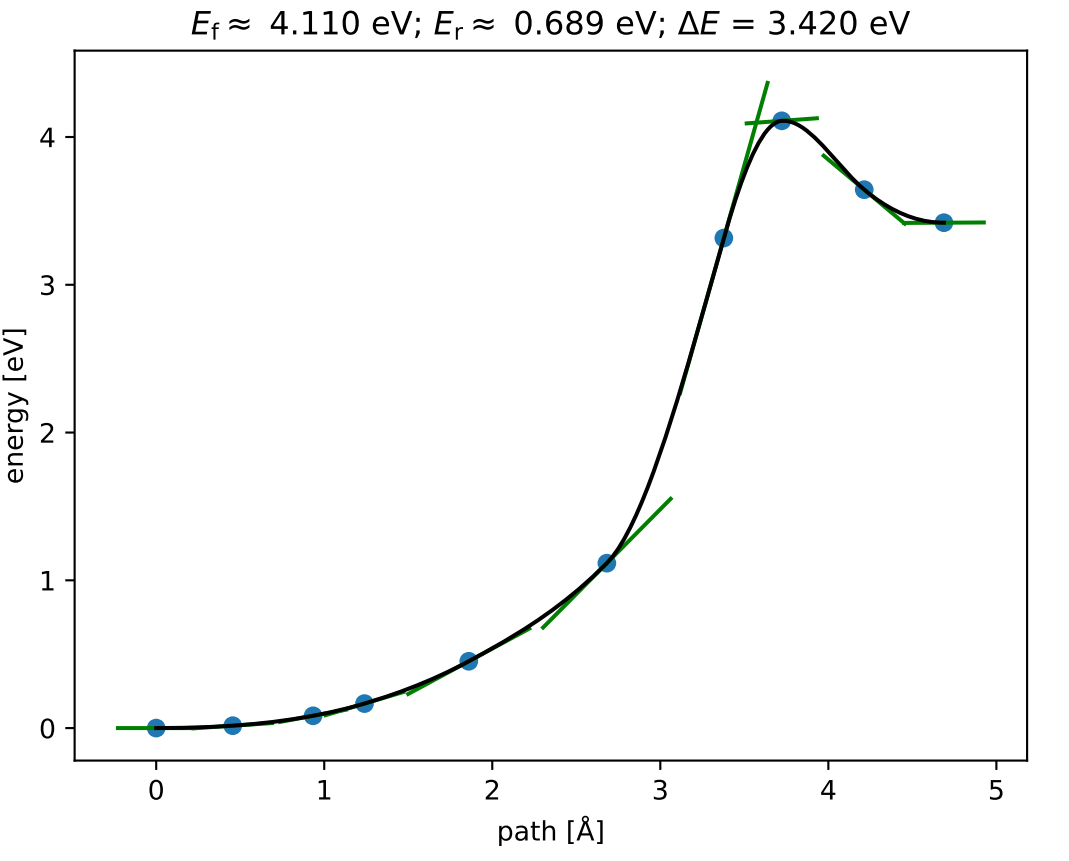
$E_f \approx$ 4.110 eV; $E_r \approx$ 0.689 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
1
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4
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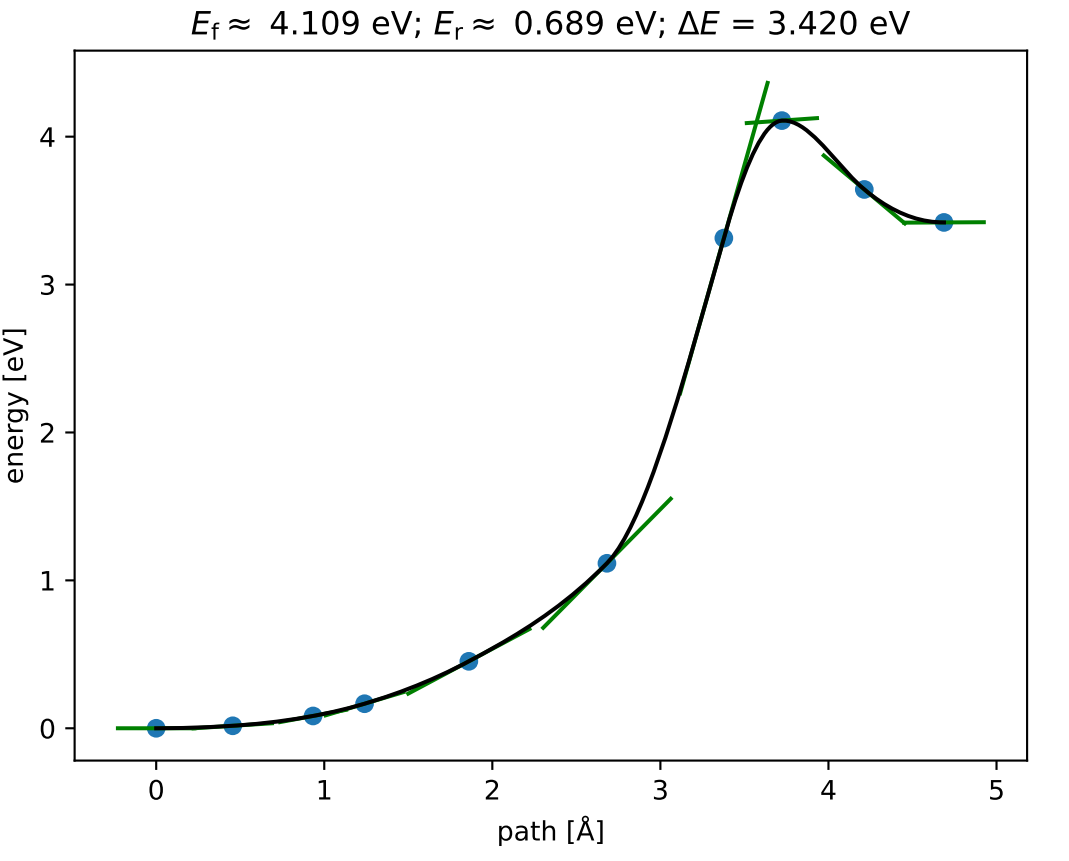
$E_f \approx$ 4.109 eV; $E_r \approx$ 0.689 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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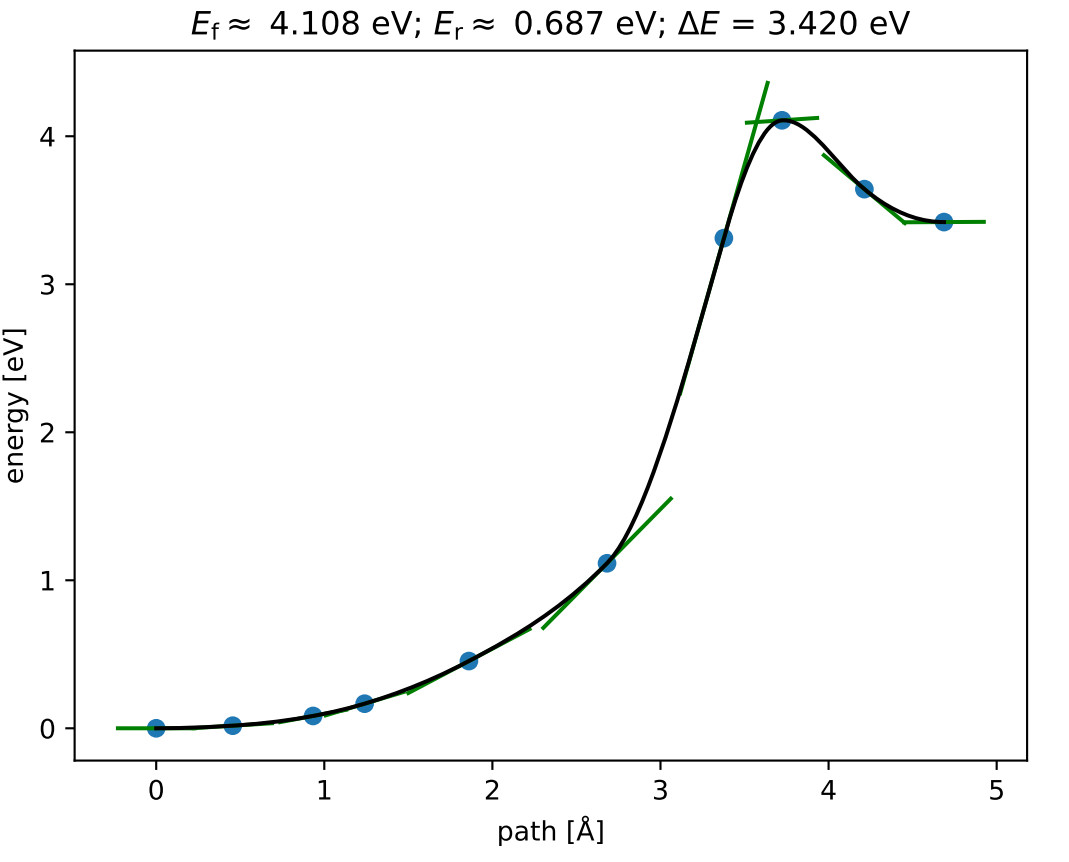
4
5


$E_f \approx$ 4.108 eV; $E_r \approx$ 0.687 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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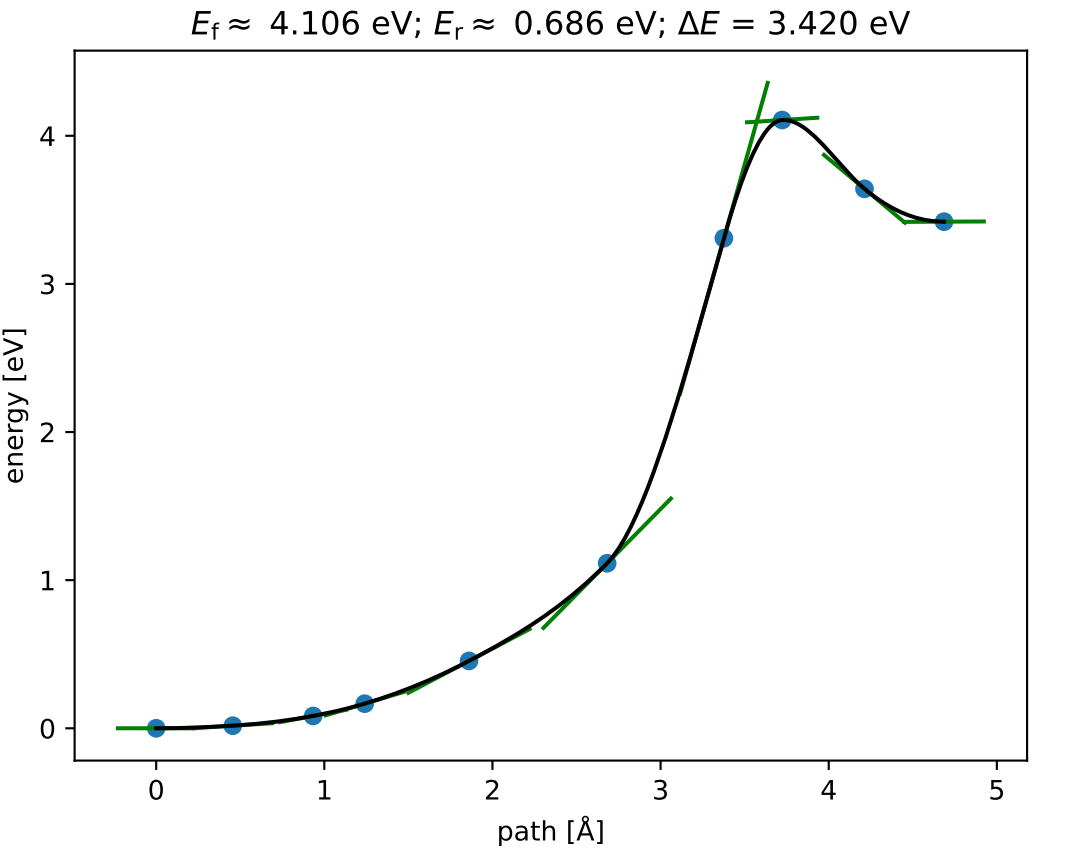
$E_f \approx$ 4.106 eV; $E_r \approx$ 0.686 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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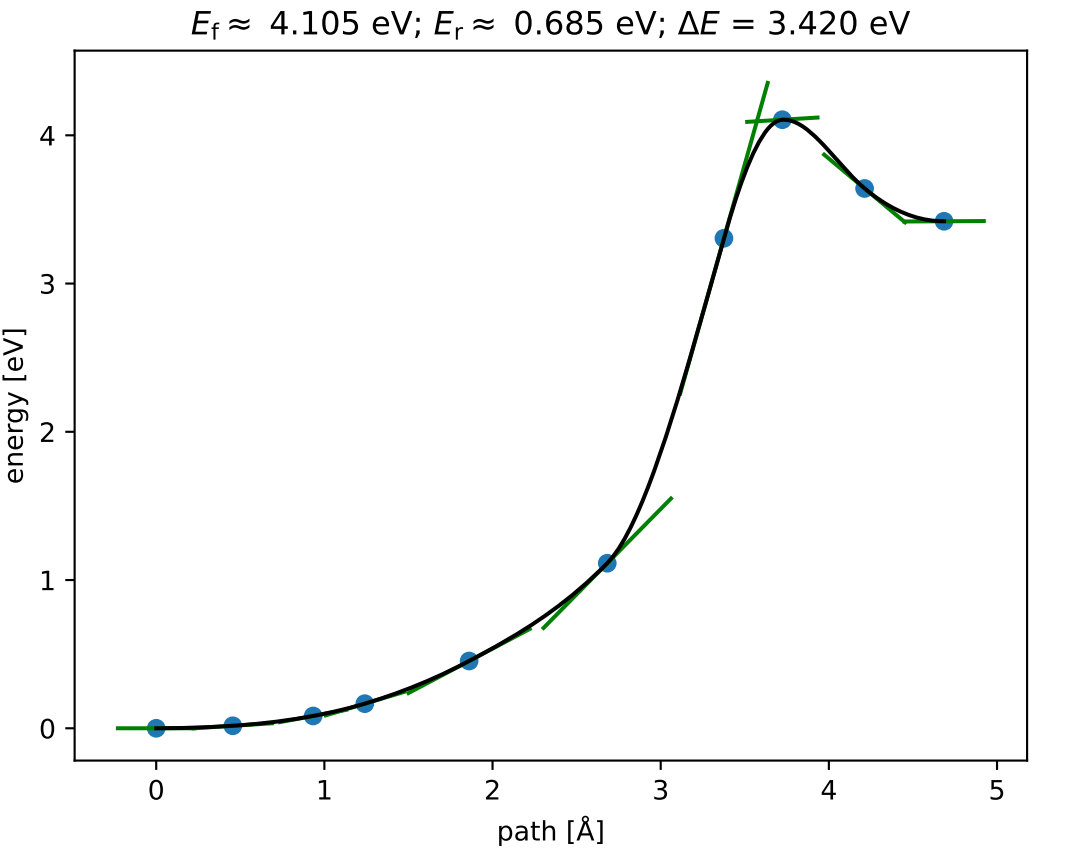
$E_f \approx$ 4.105 eV; $E_r \approx$ 0.685 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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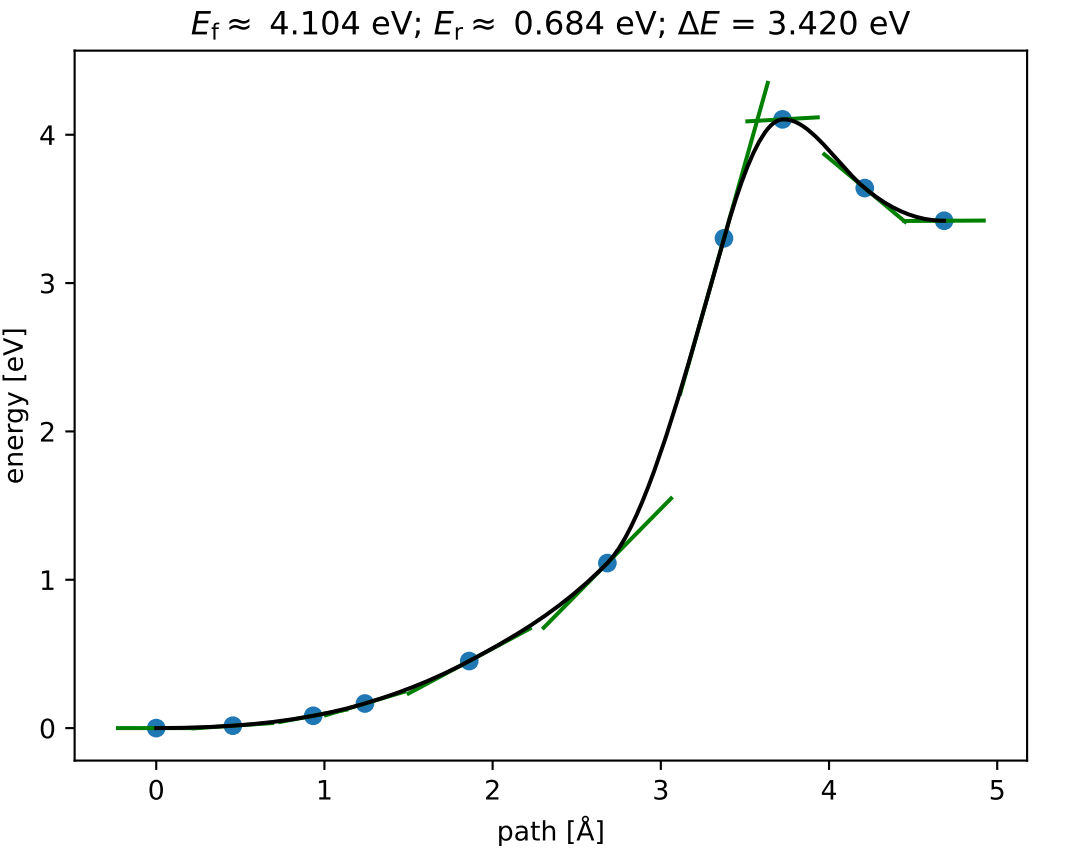
$E_f \approx$ 4.104 eV; $E_r \approx$ 0.684 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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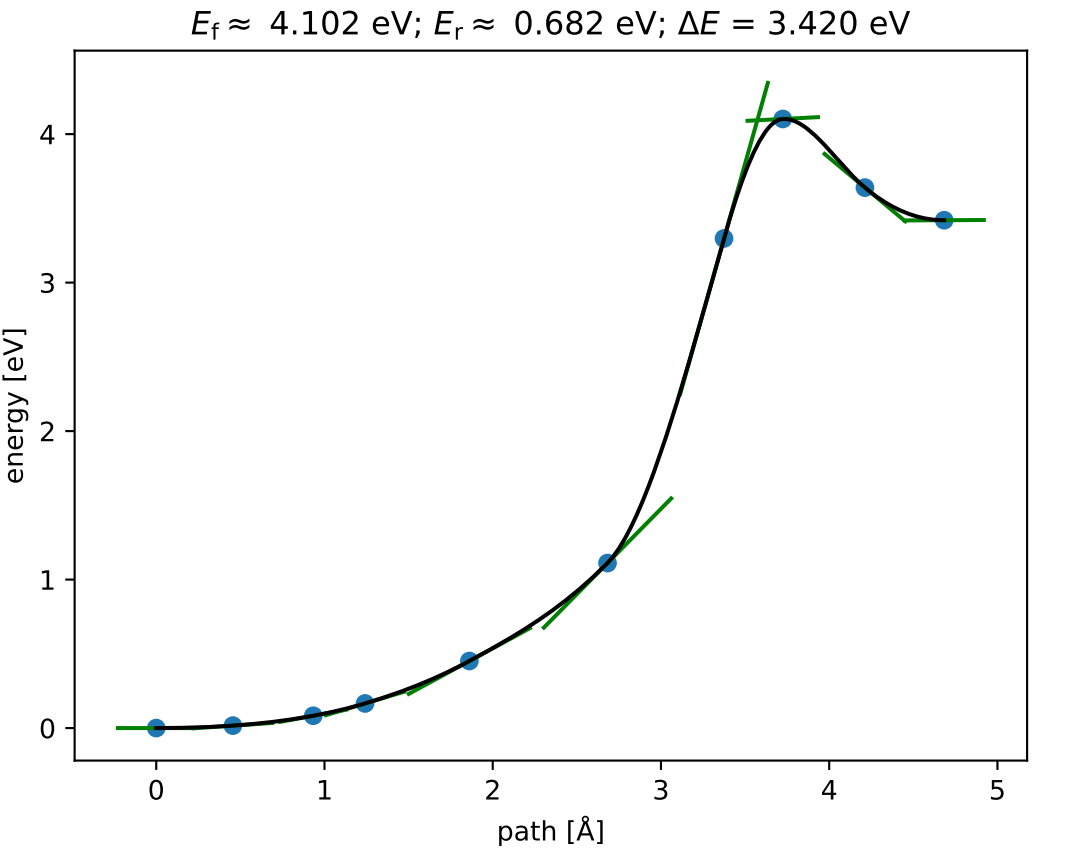
$E_f \approx$ 4.102 eV; $E_r \approx$ 0.682 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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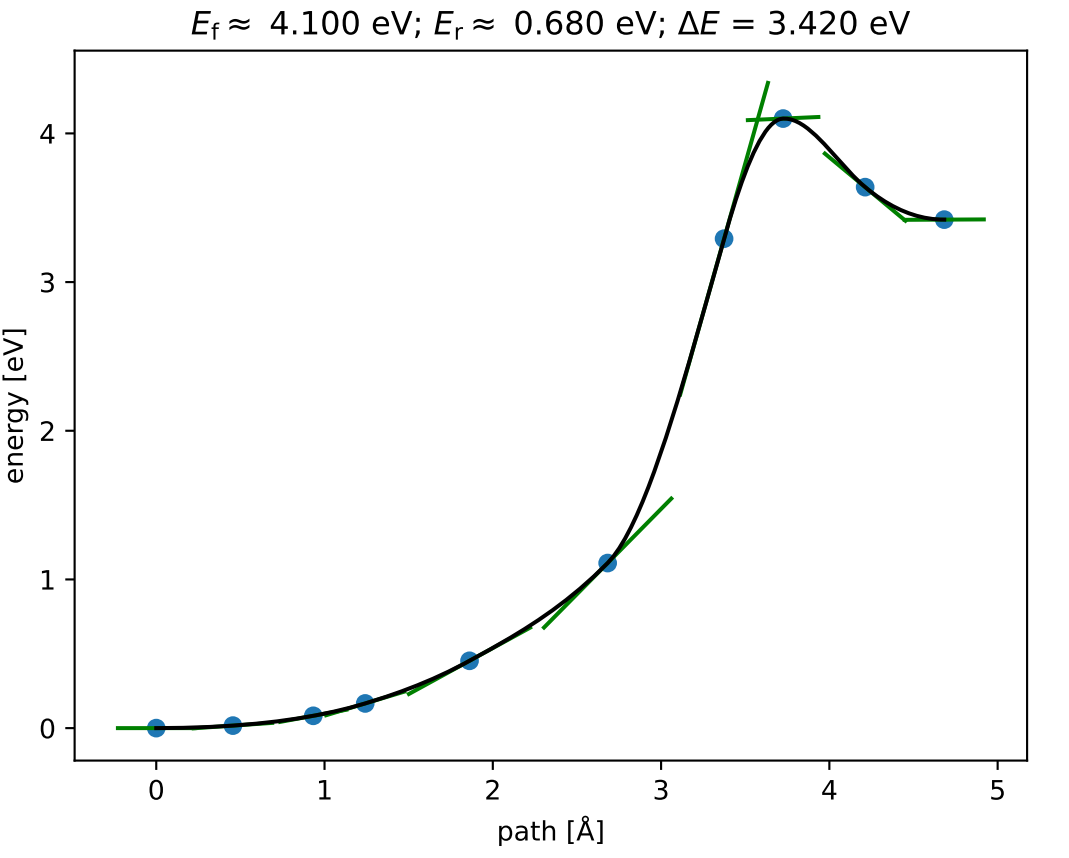
$E_f \approx$ 4.100 eV; $E_r \approx$ 0.680 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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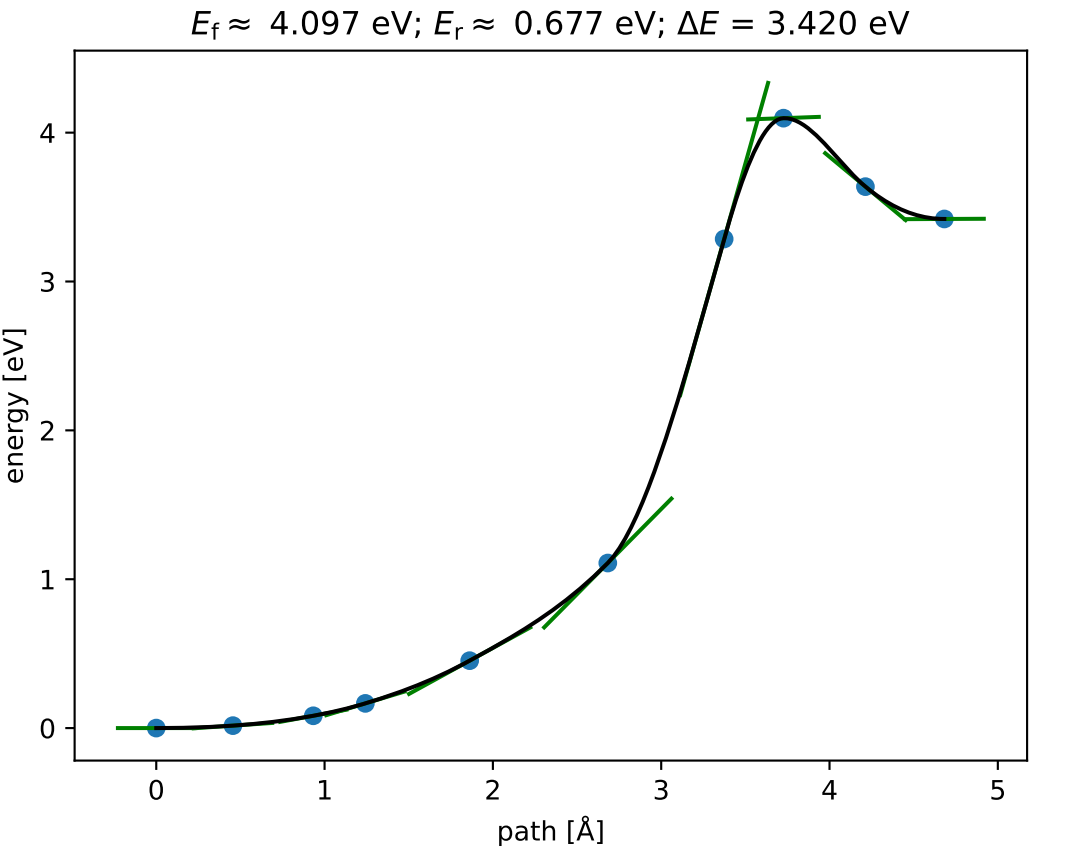
$E_f \approx$ 4.097 eV; $E_r \approx$ 0.677 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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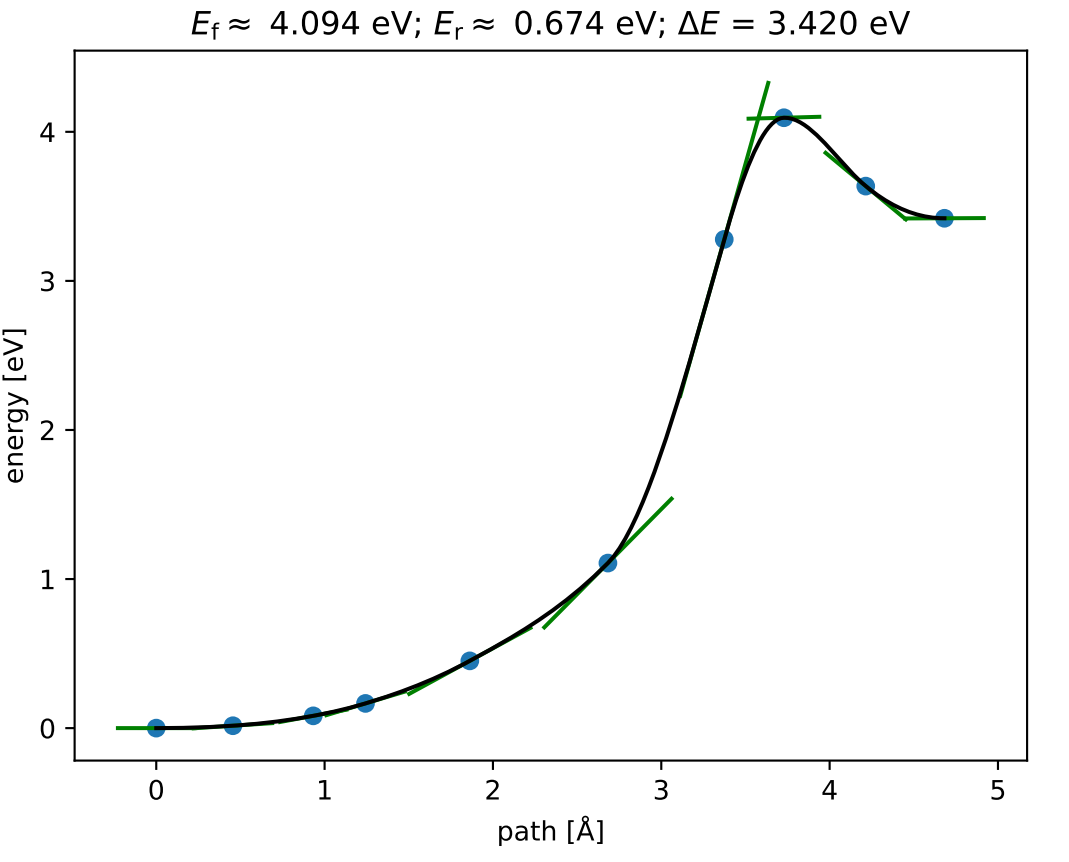
$E_f \approx$ 4.094 eV; $E_r \approx$ 0.674 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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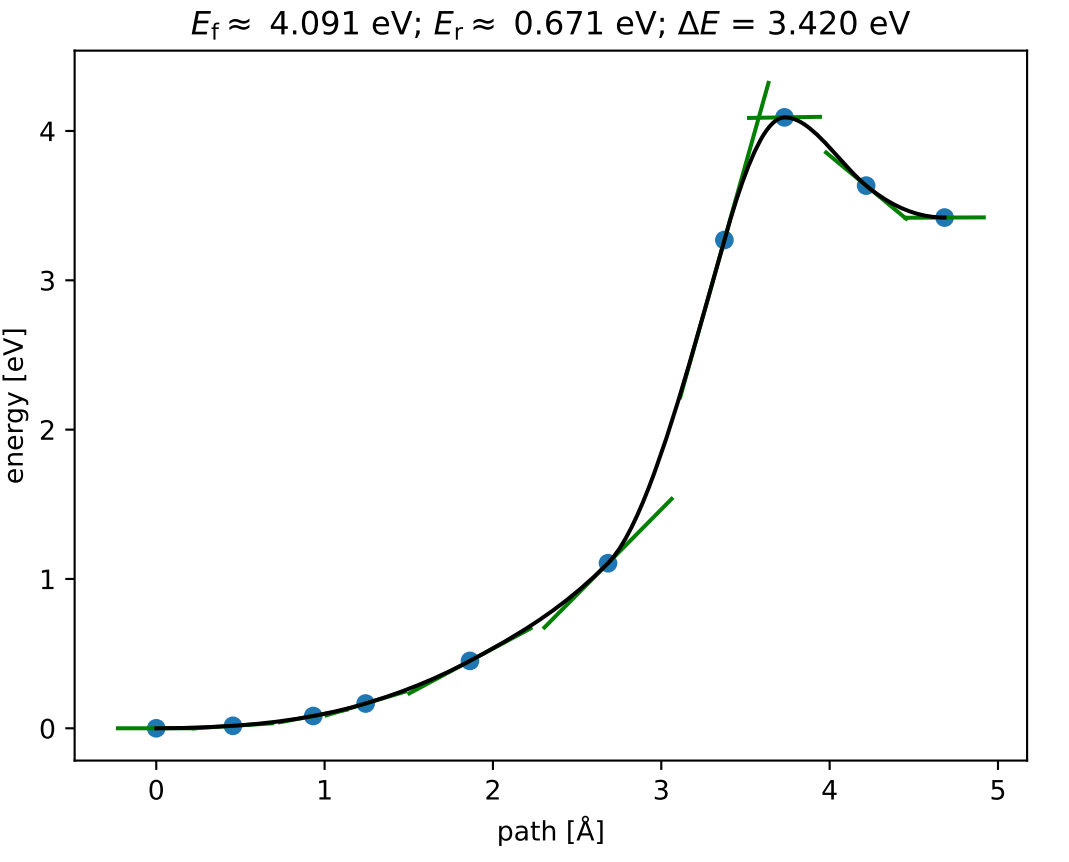
$E_f \approx$ 4.091 eV; $E_r \approx$ 0.671 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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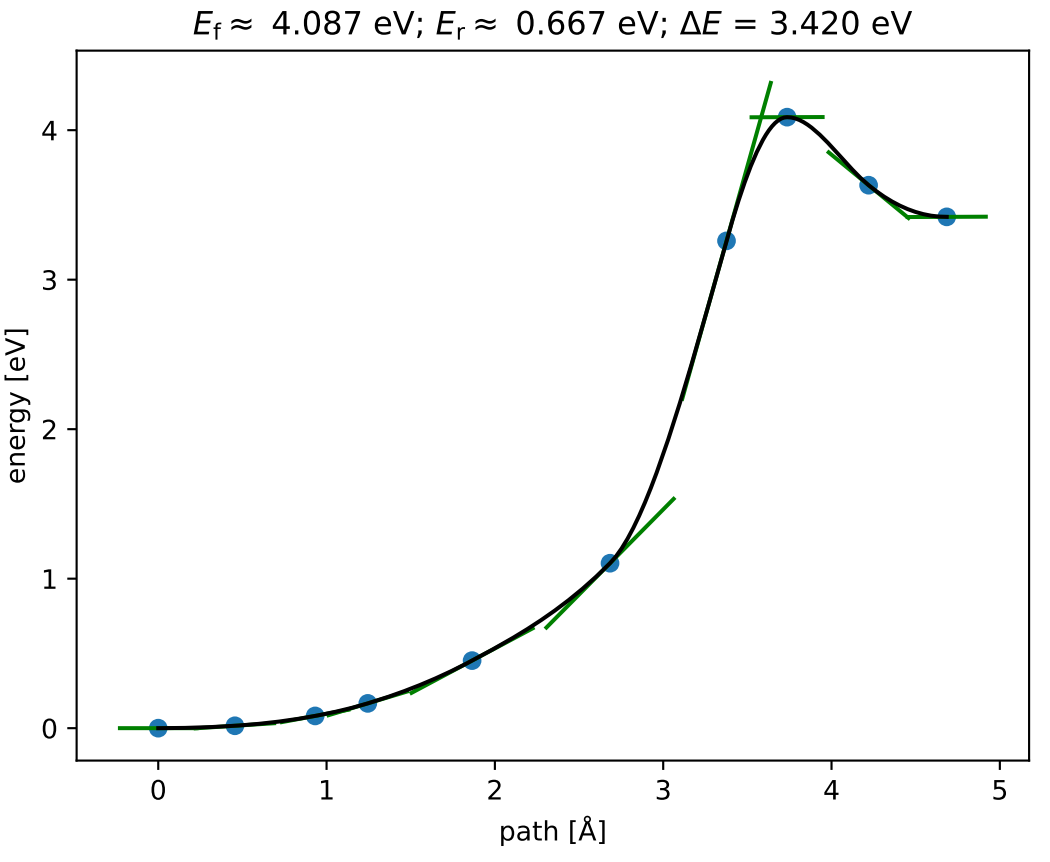
$E_f \approx$ 4.087 eV; $E_r \approx$ 0.667 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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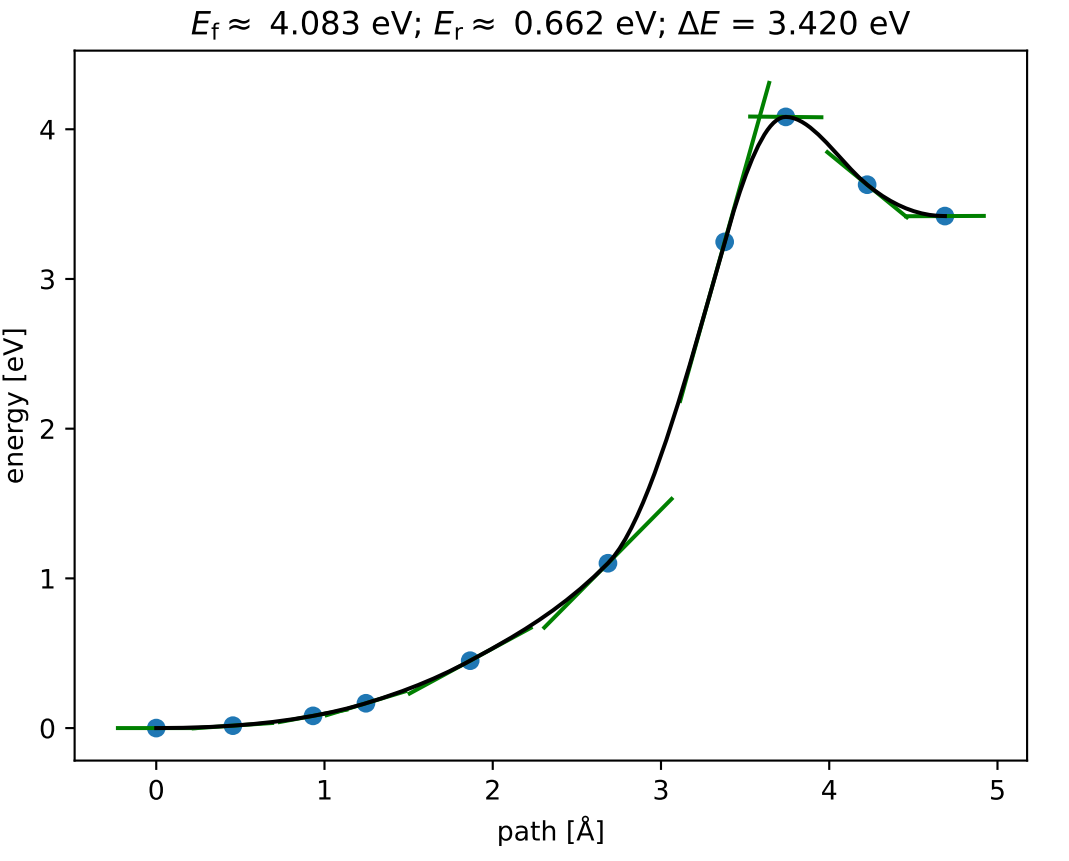
$E_f \approx$ 4.083 eV; $E_r \approx$ 0.662 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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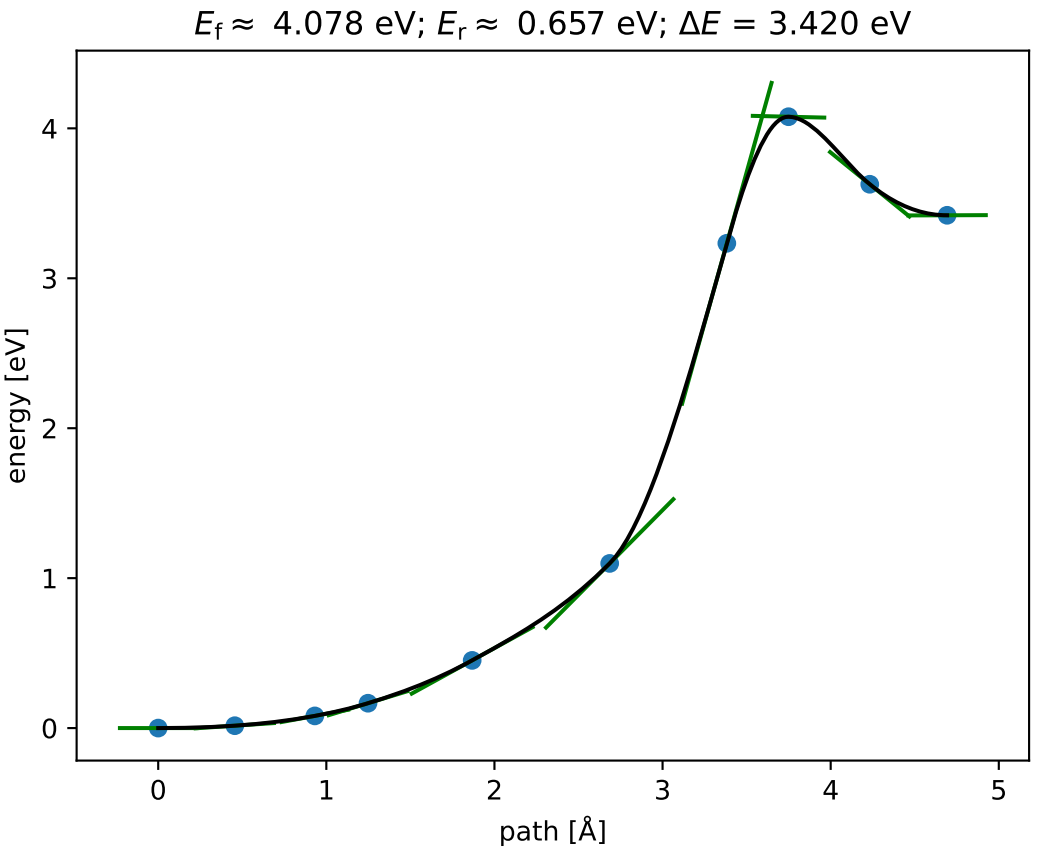
$E_f \approx$ 4.078 eV; $E_r \approx$ 0.657 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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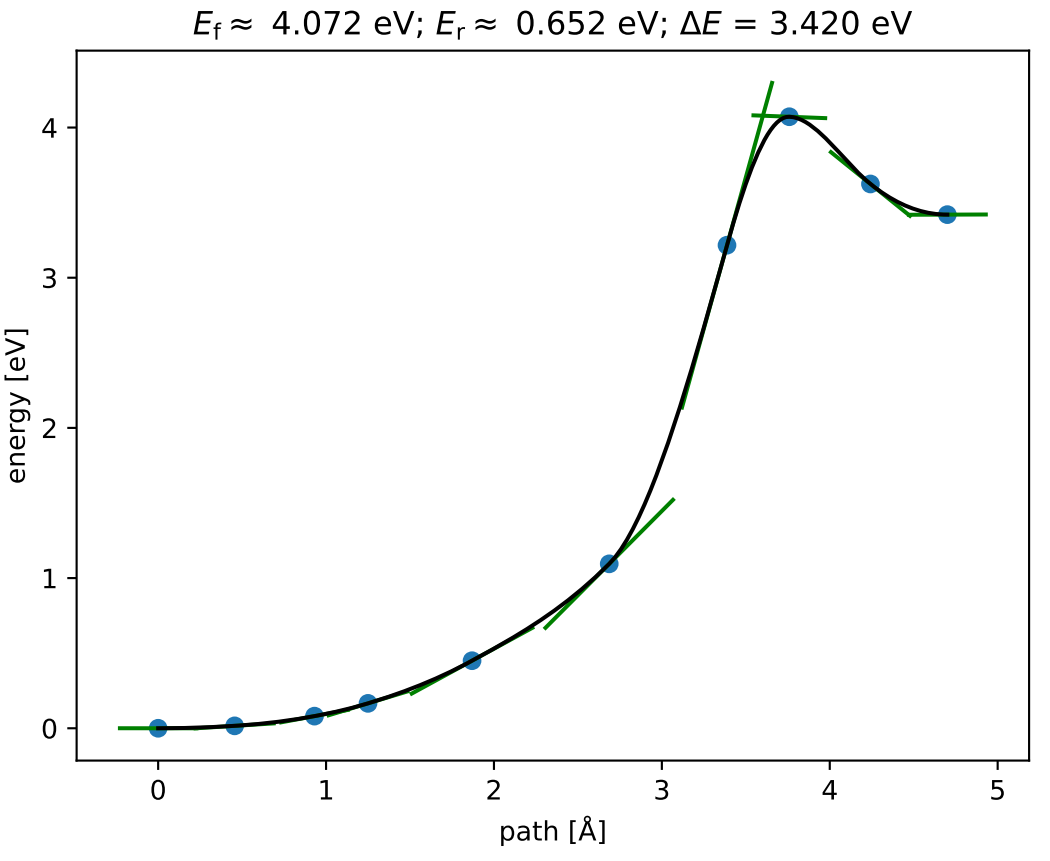
$E_f \approx$ 4.072 eV; $E_r \approx$ 0.652 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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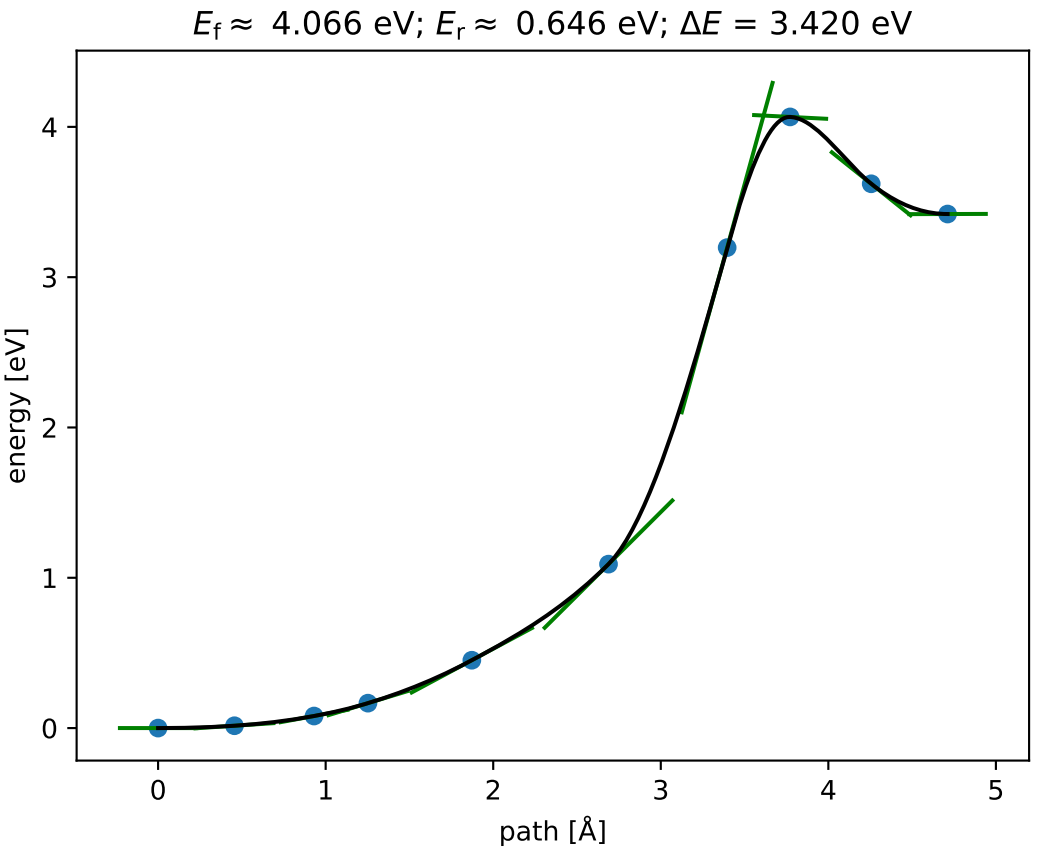
$E_f \approx$ 4.066 eV; $E_r \approx$ 0.646 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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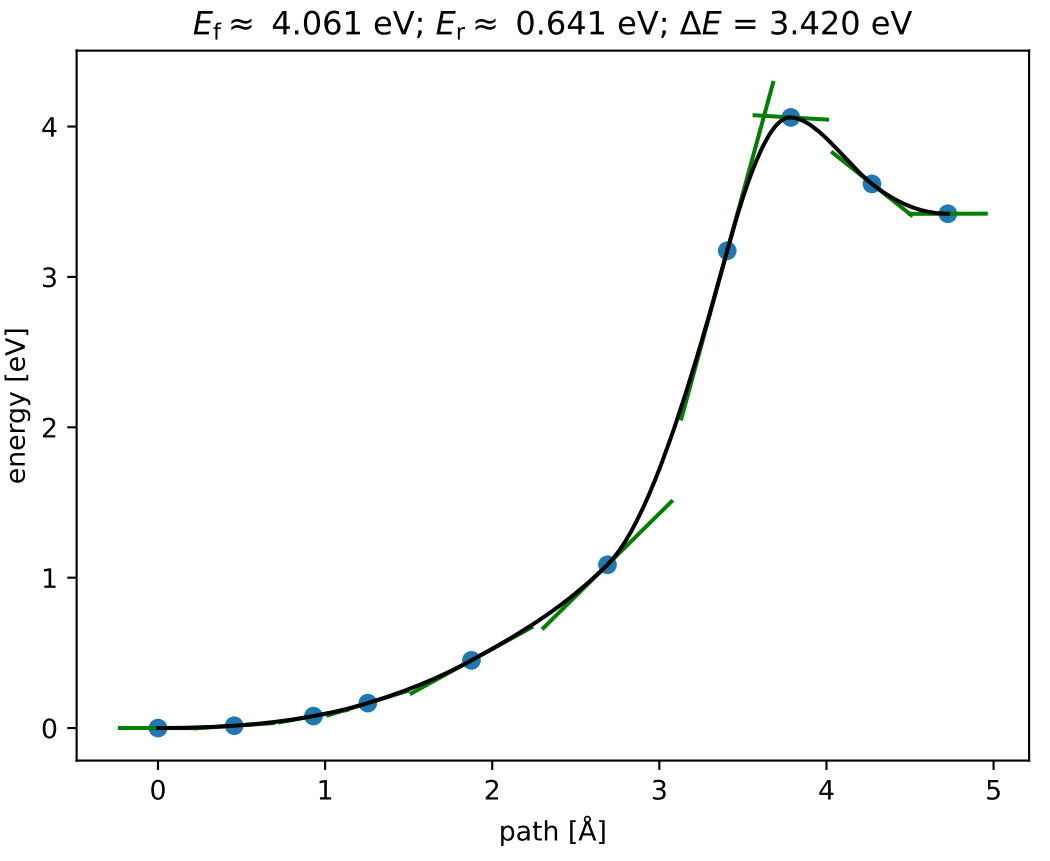
$E_f \approx$ 4.061 eV; $E_r \approx$ 0.641 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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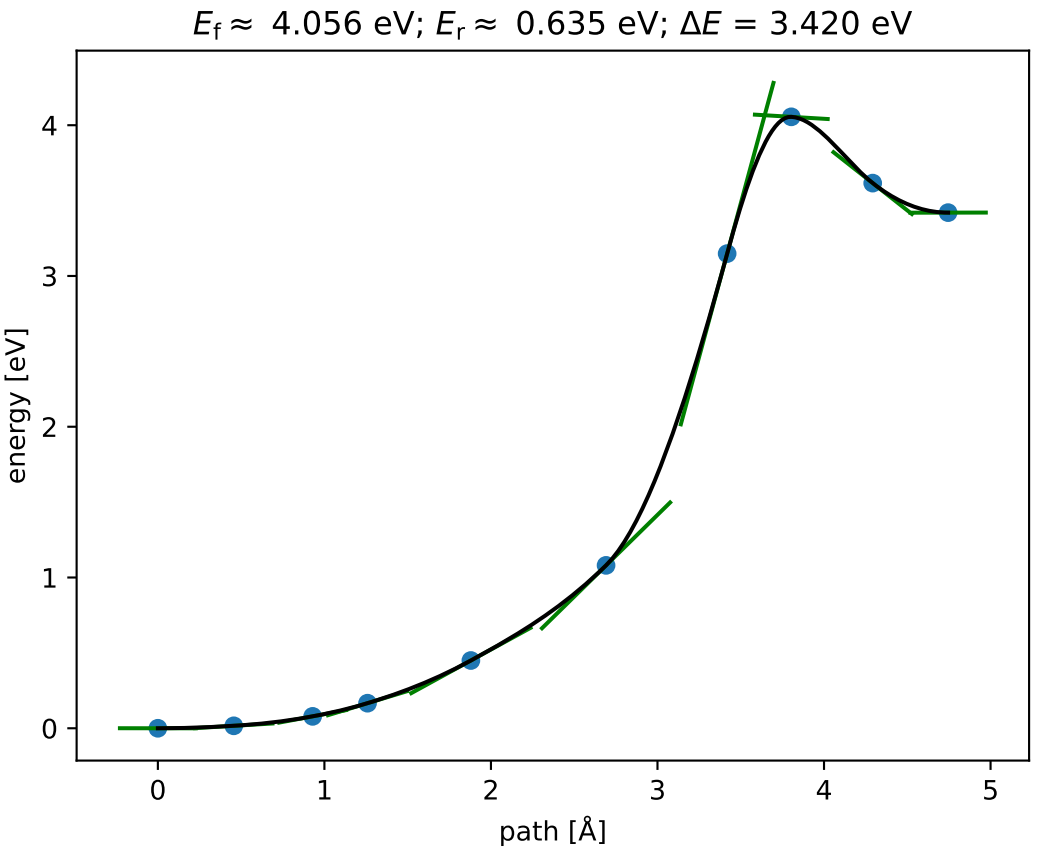
$E_f \approx$ 4.056 eV; $E_r \approx$ 0.635 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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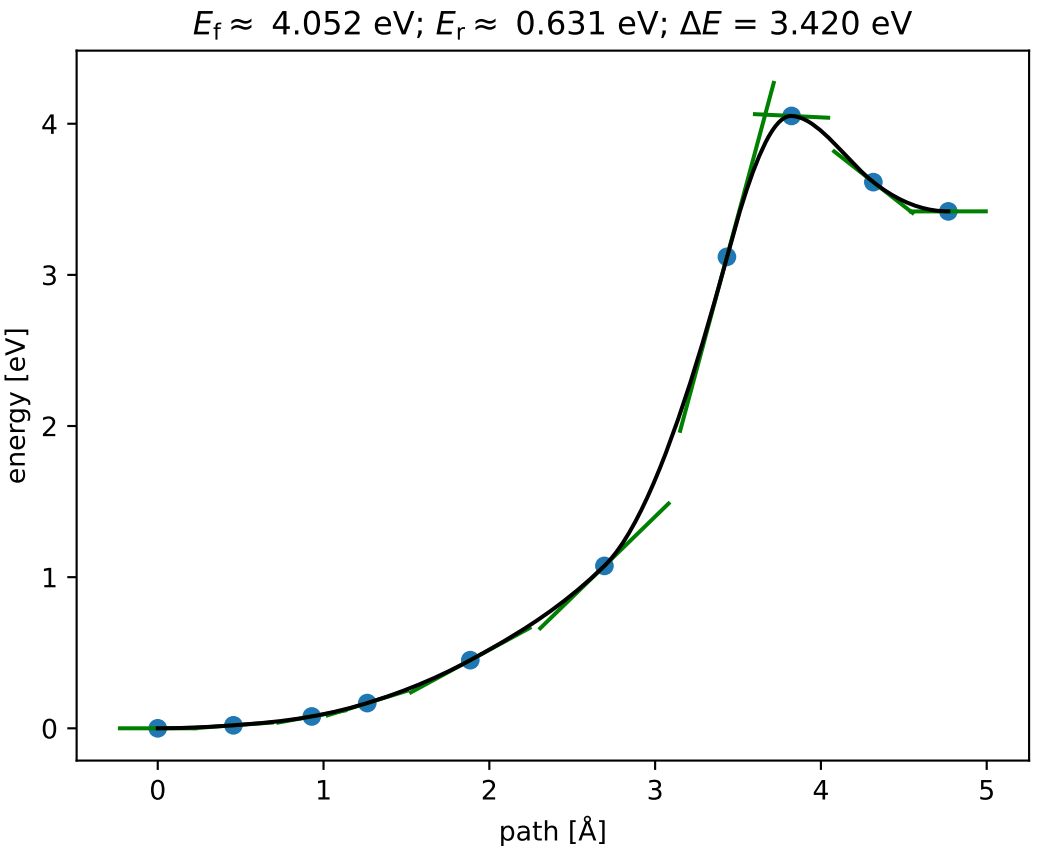
$E_f \approx$ 4.052 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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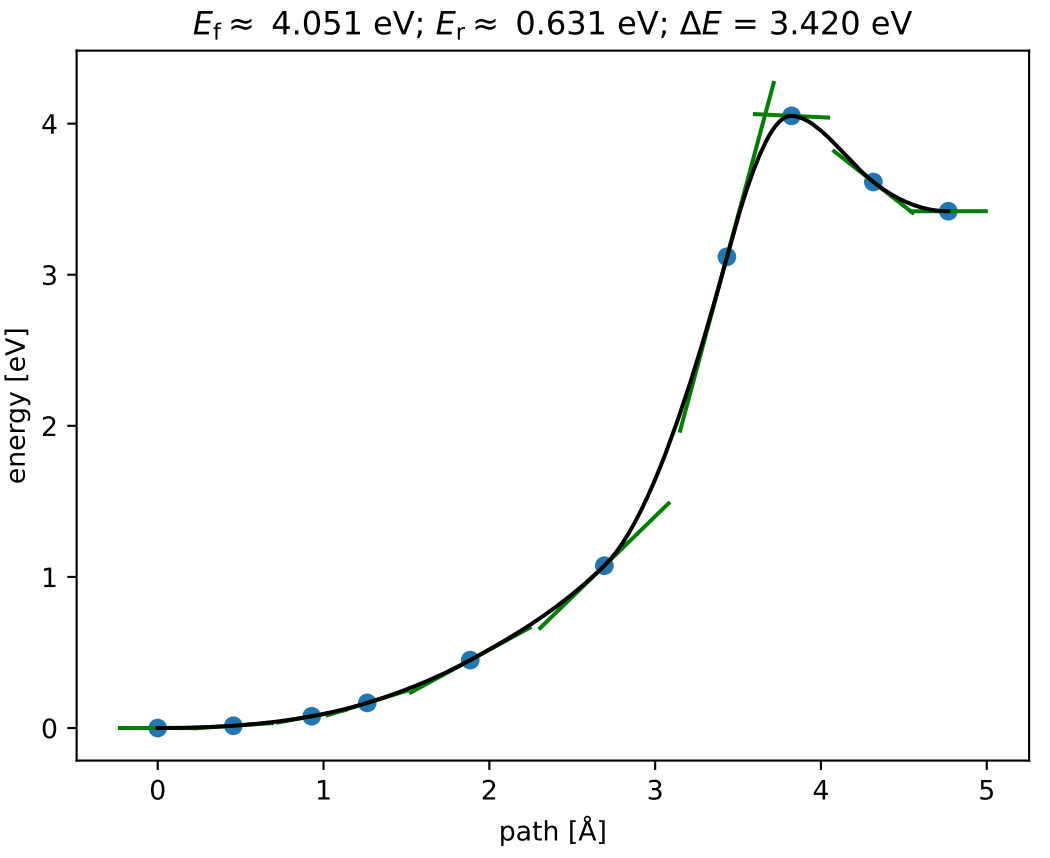
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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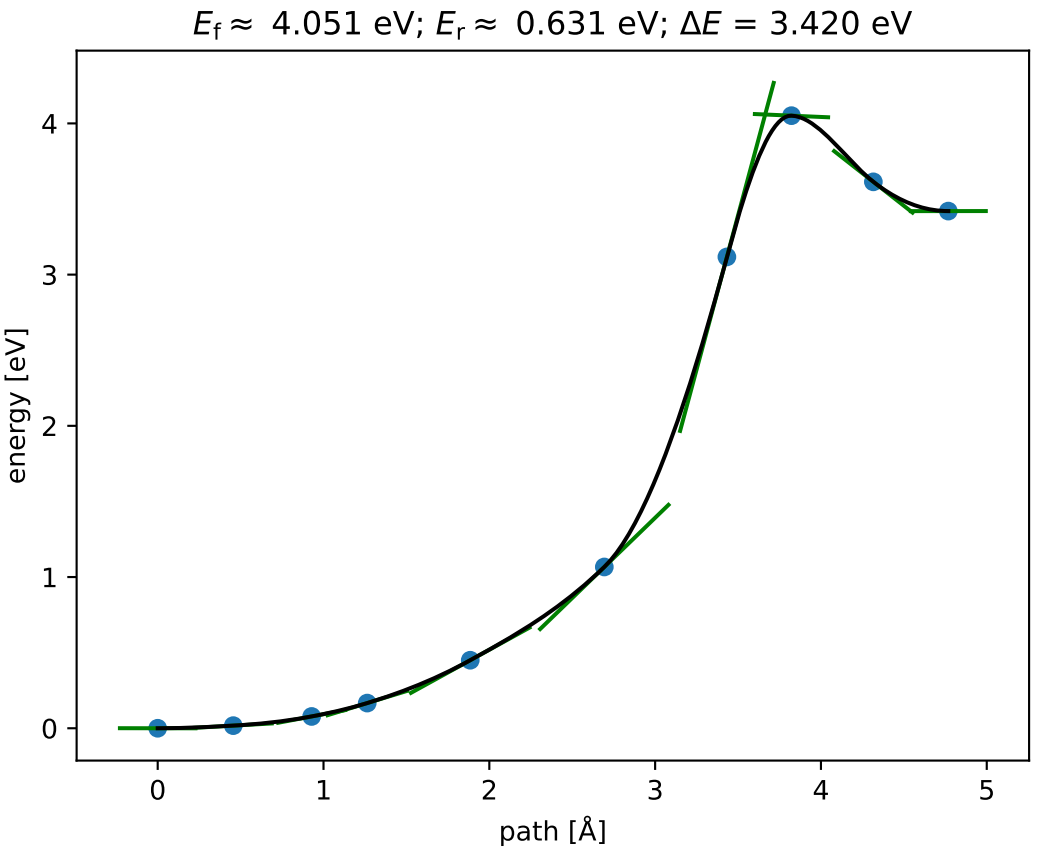
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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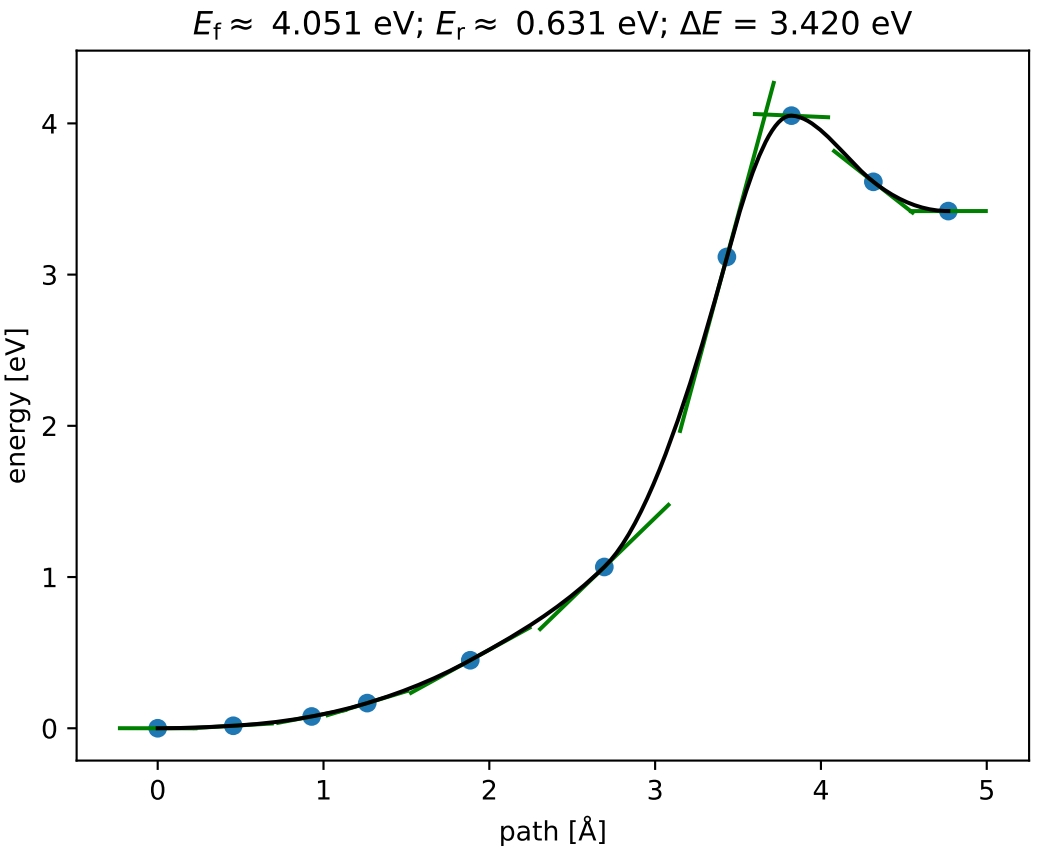
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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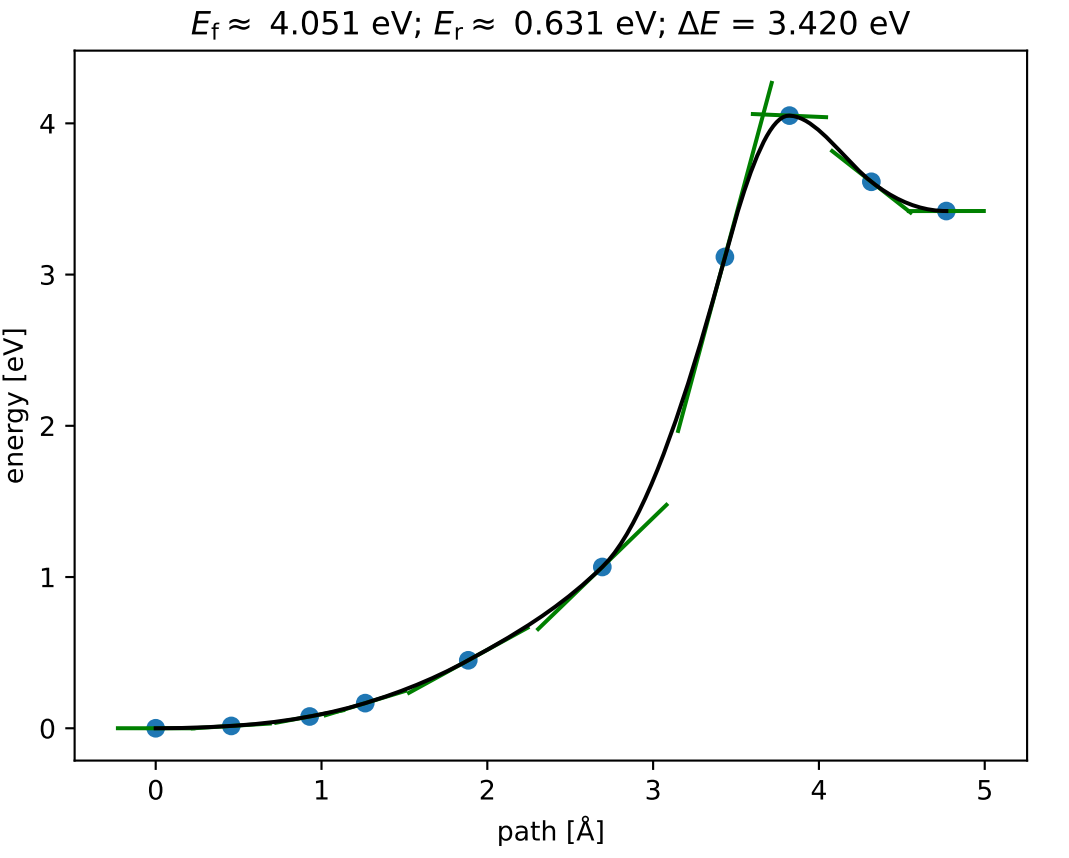
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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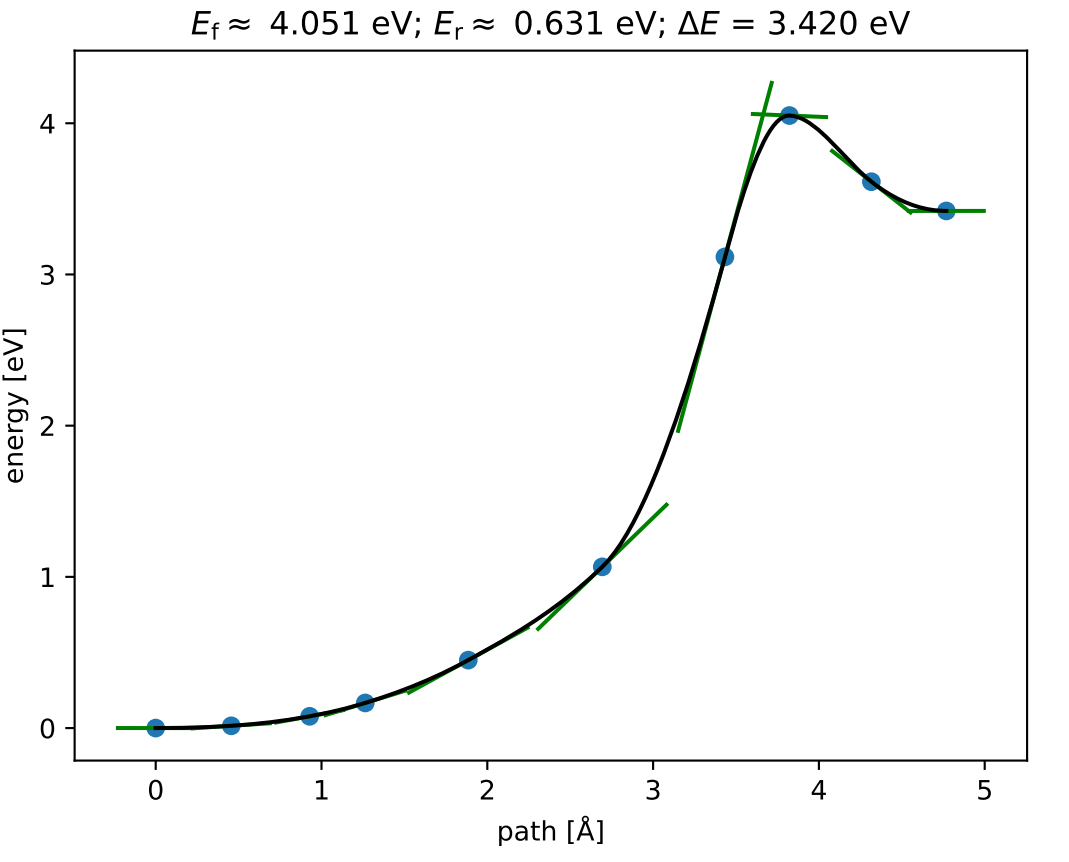
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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4
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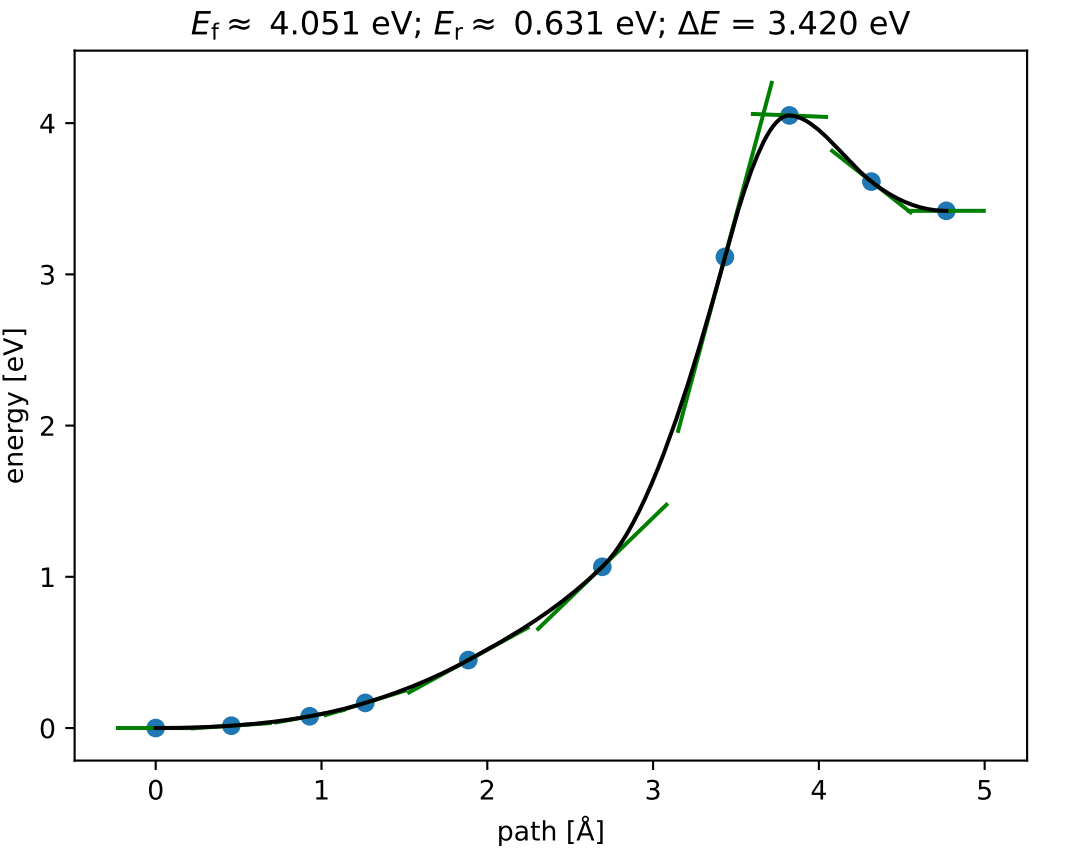
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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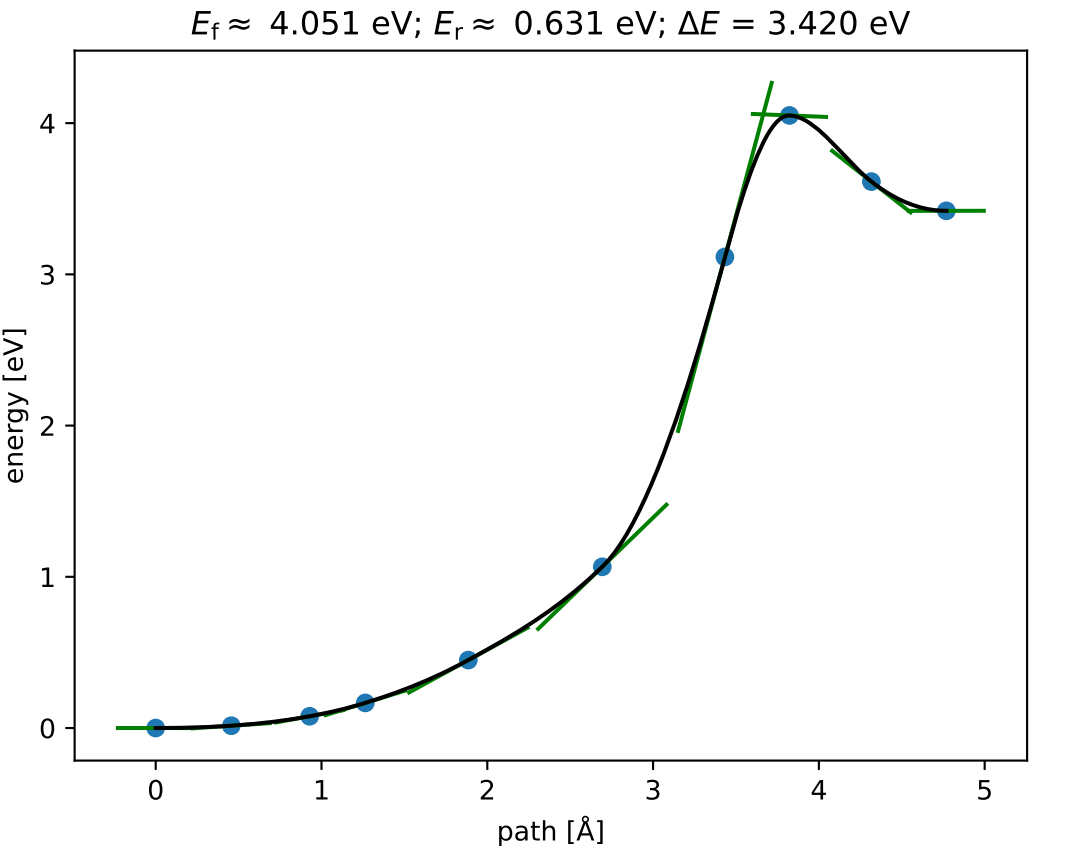
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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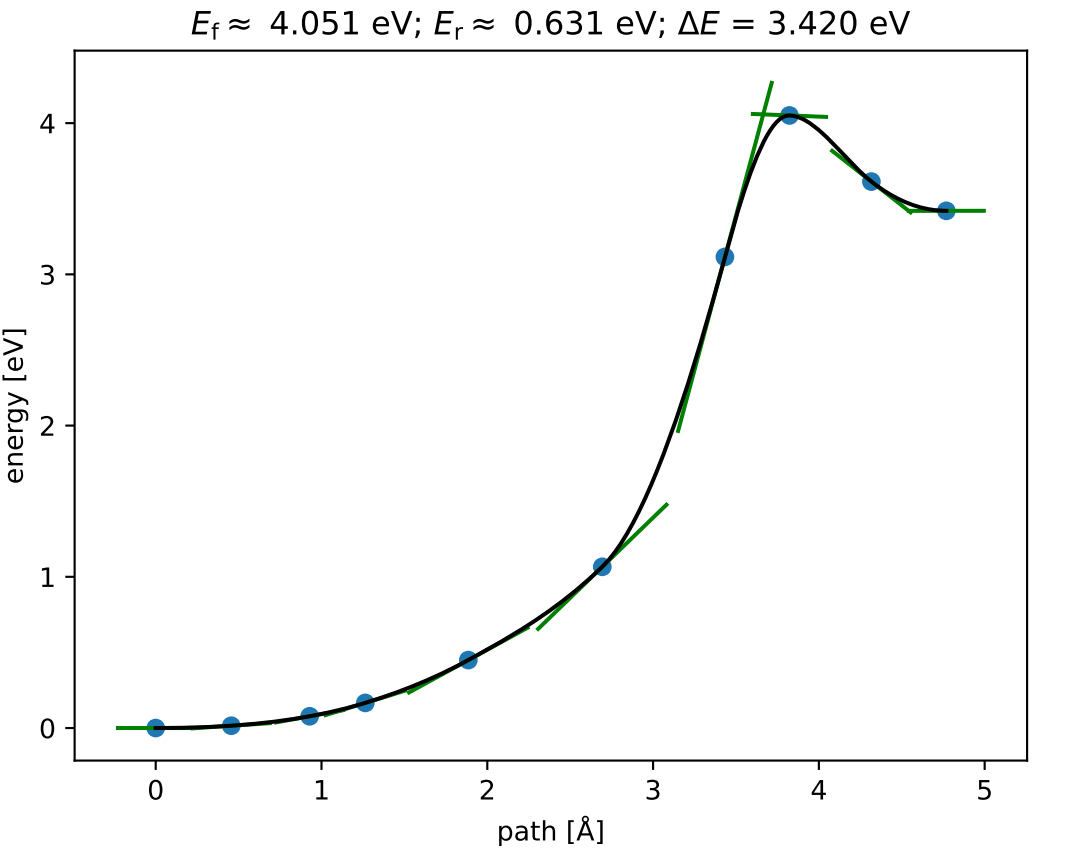
4
5


$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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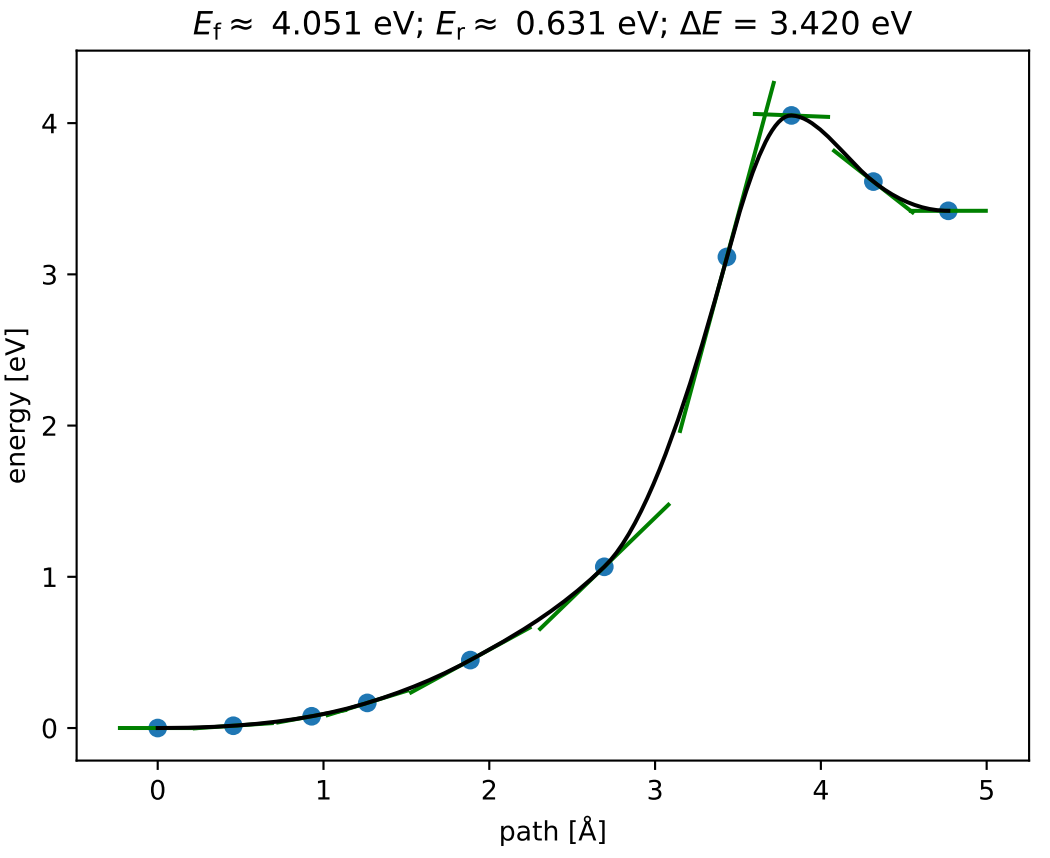
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
0
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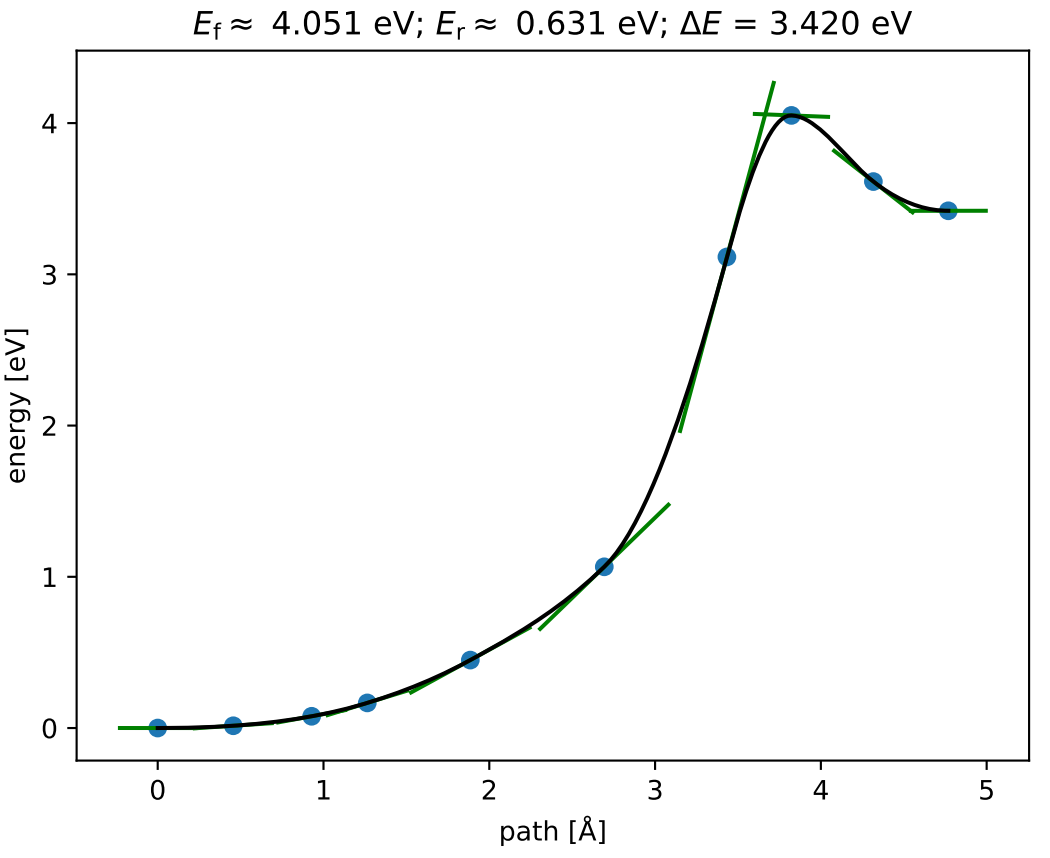
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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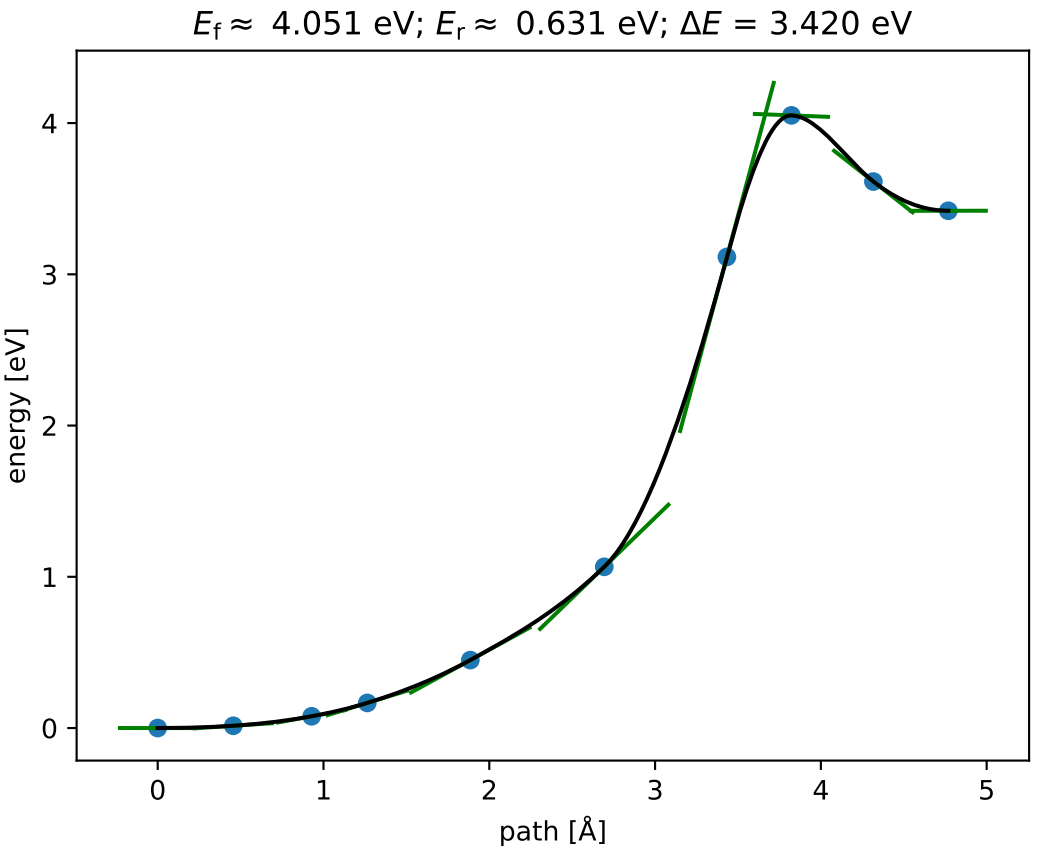
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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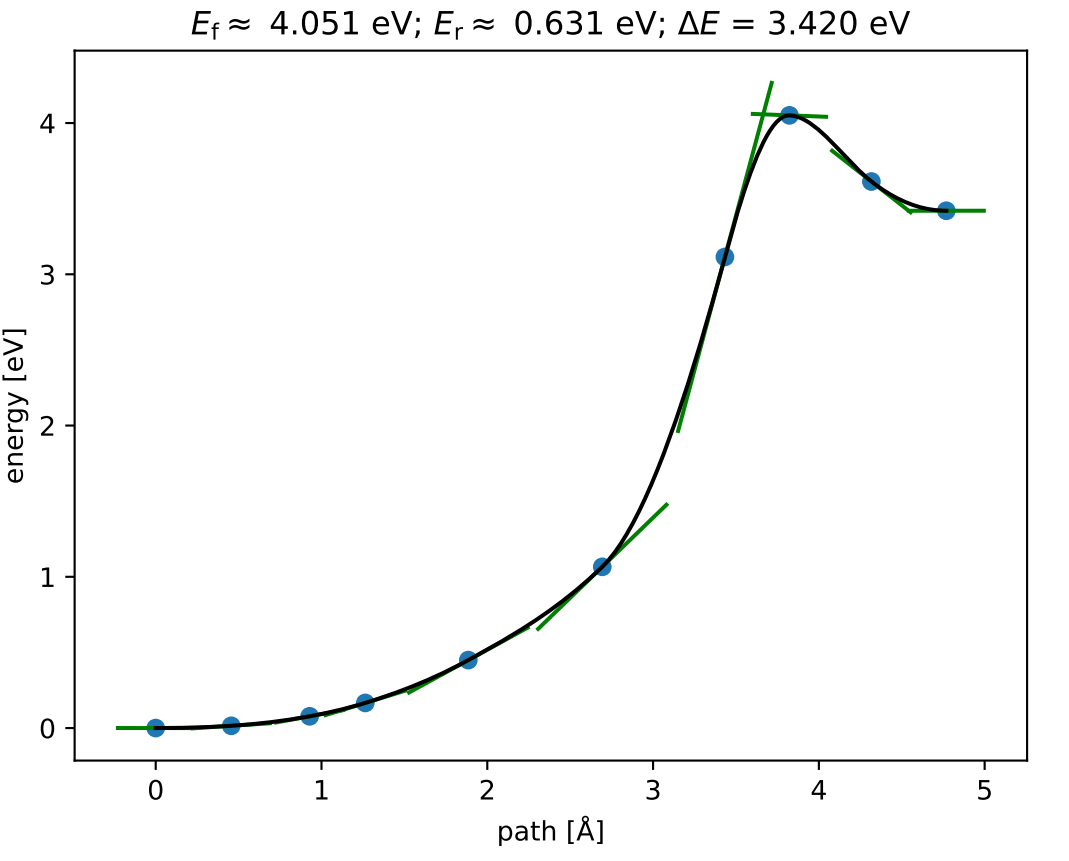
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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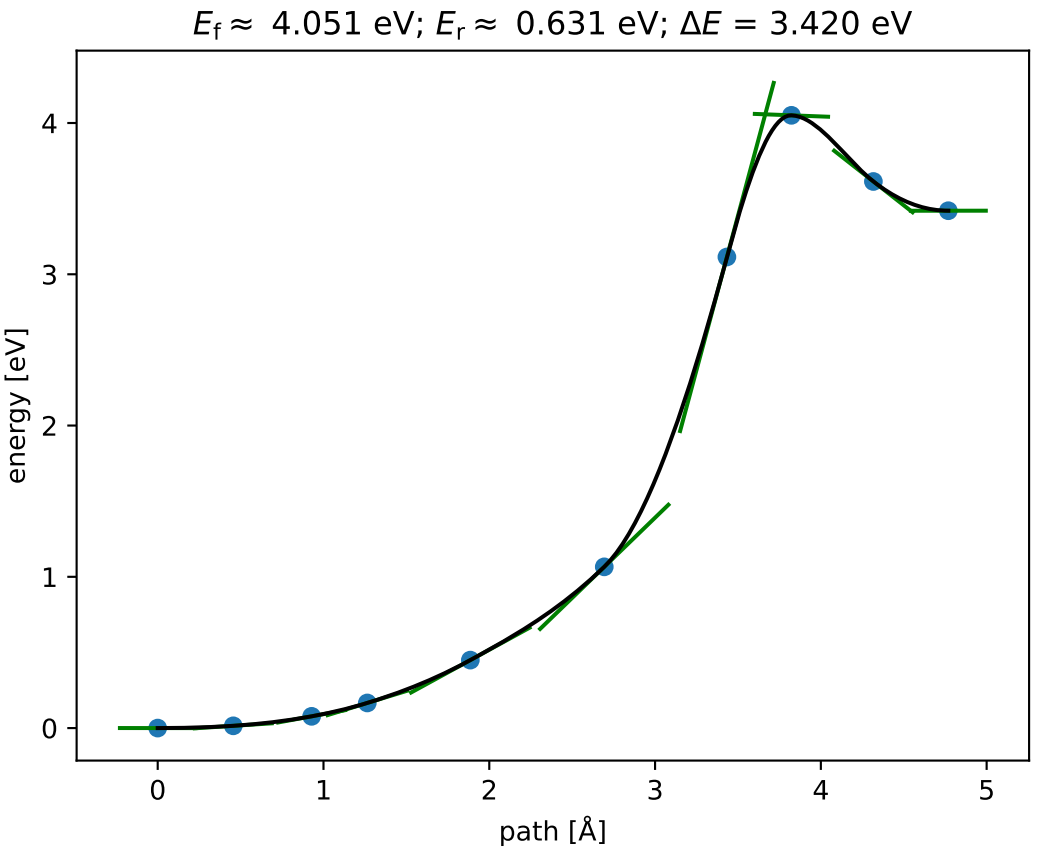
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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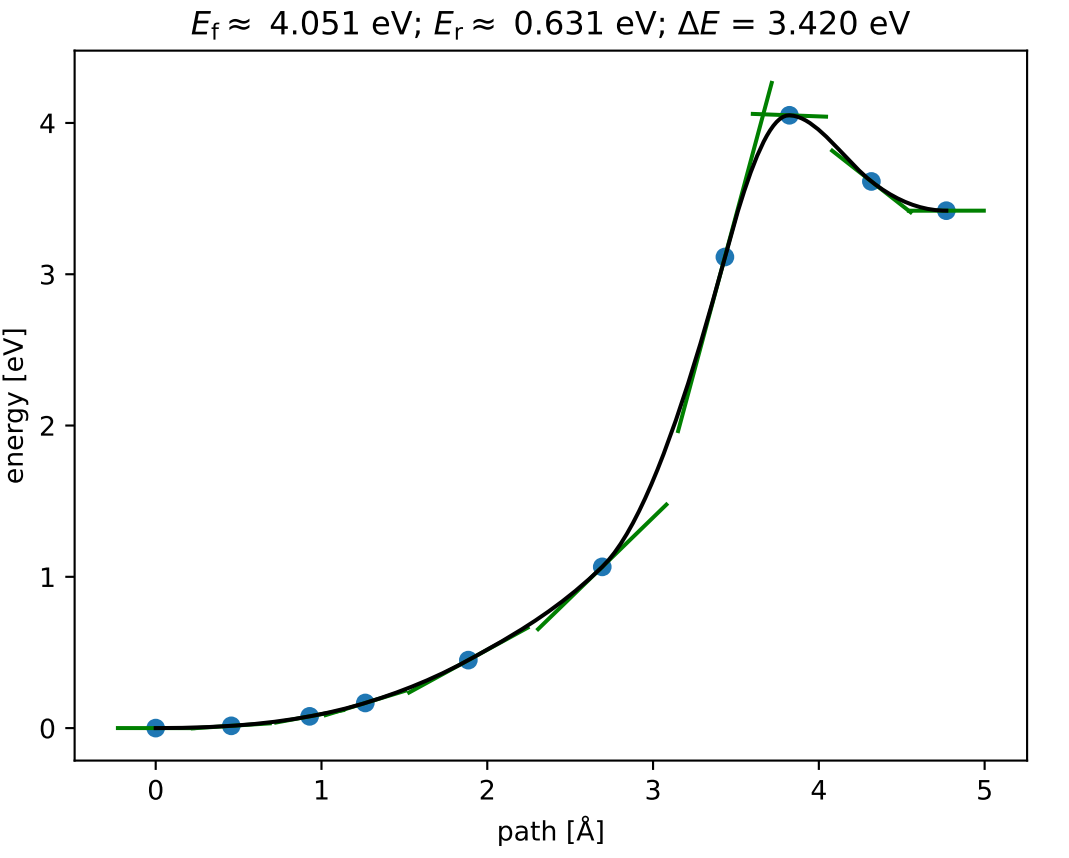
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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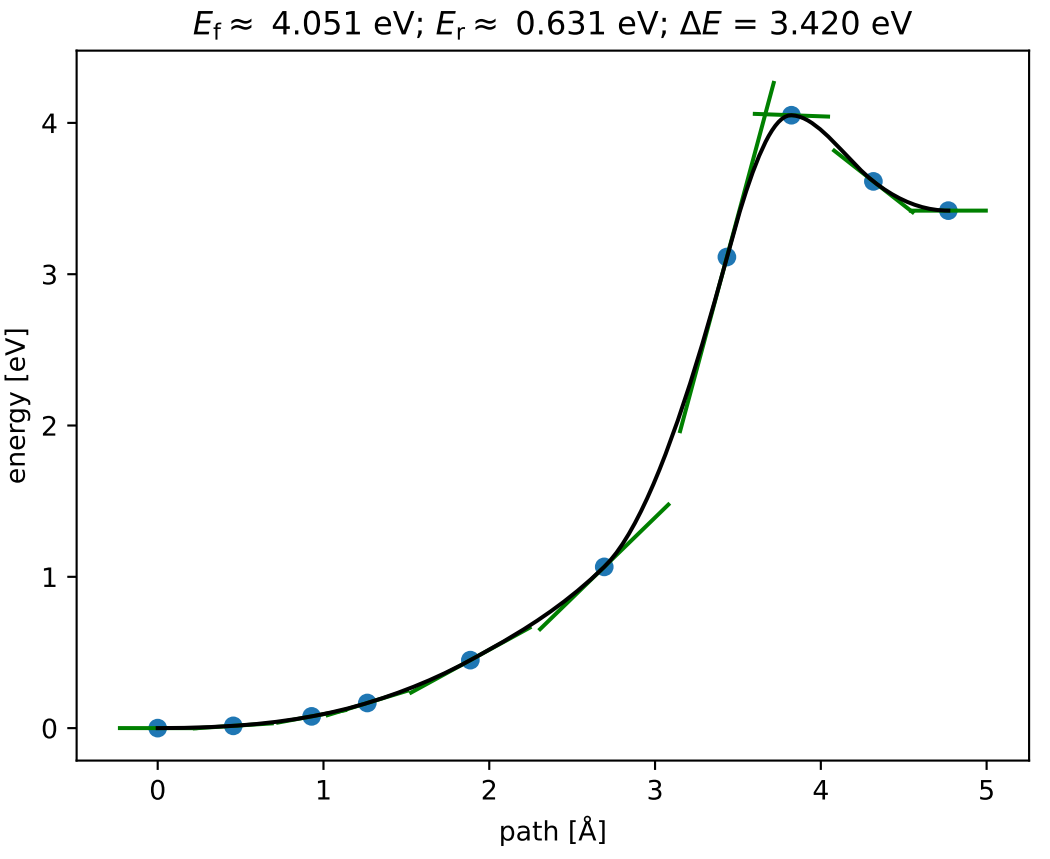
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.631 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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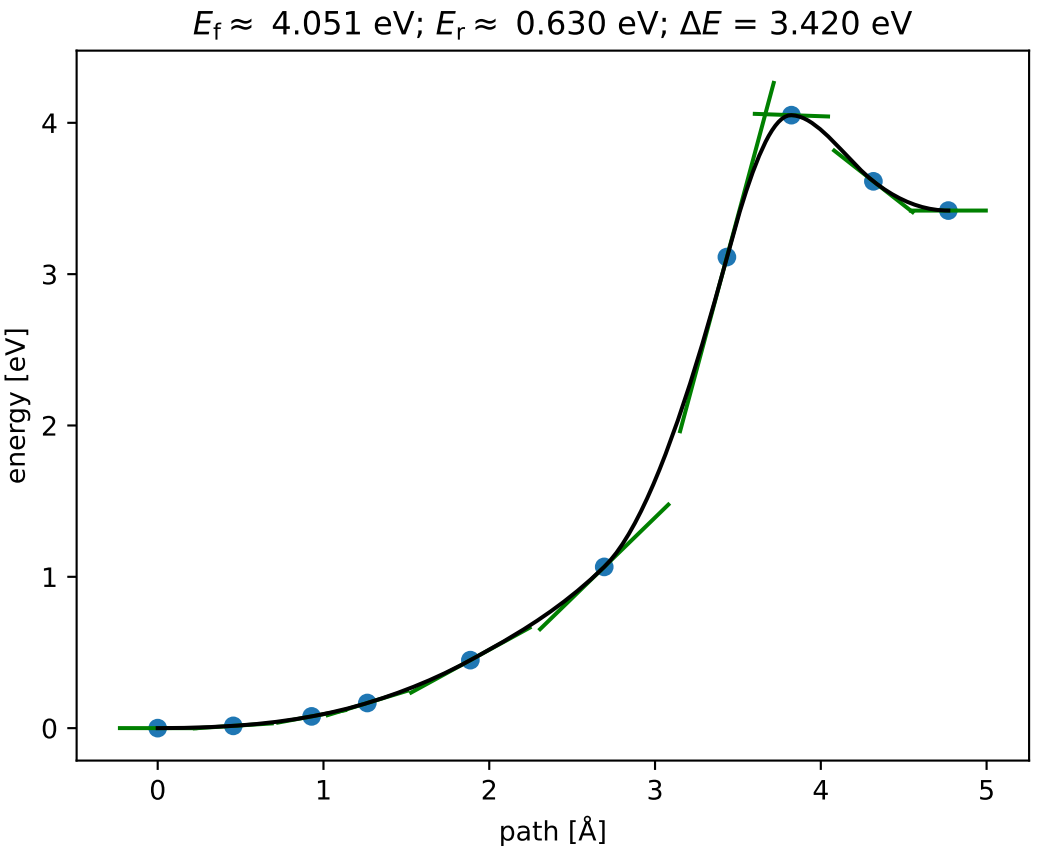
$E_f \approx$ 4.051 eV; $E_r \approx$ 0.630 eV; ΔE = 3.420 eV
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path [Å]
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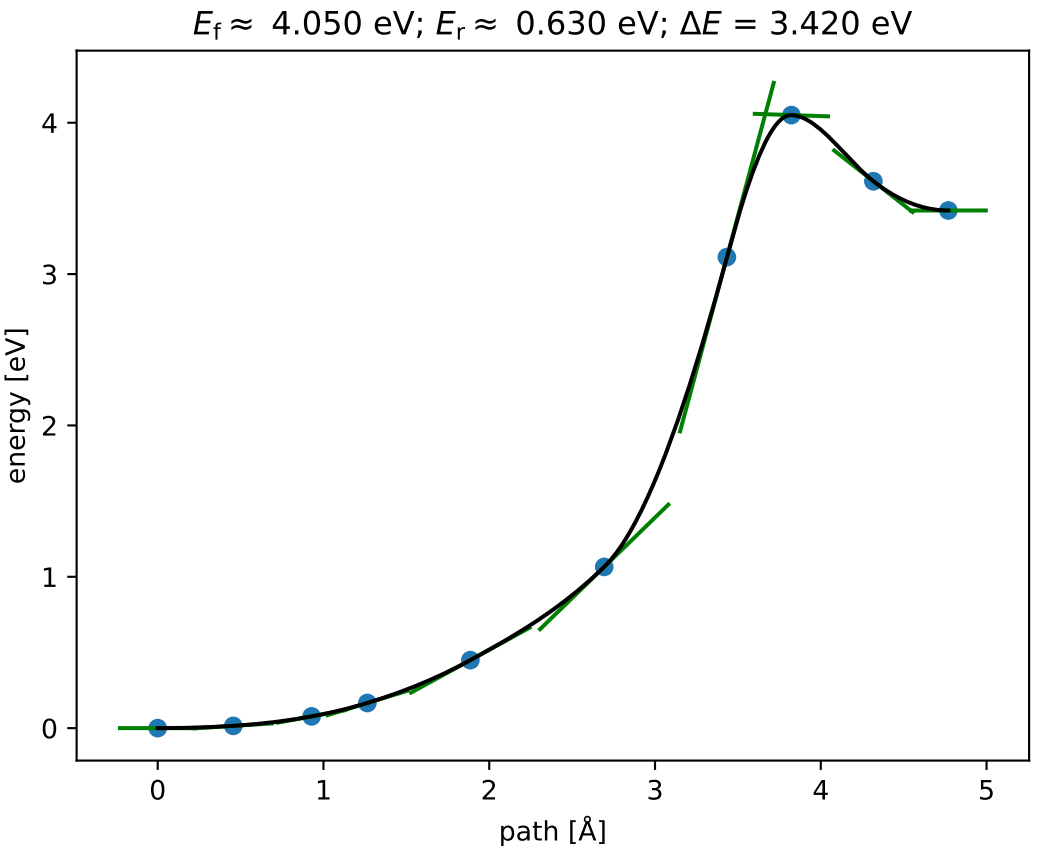
$E_f \approx$ 4.050 eV; $E_r \approx$ 0.630 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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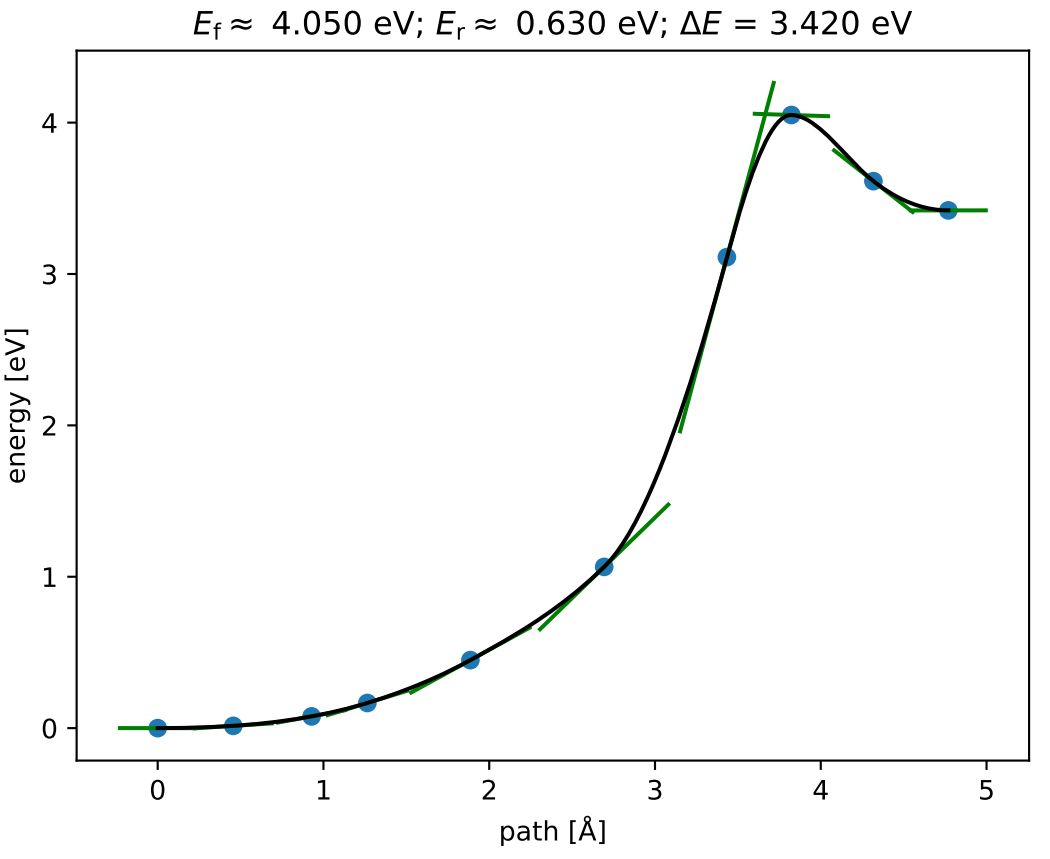
$E_f \approx$ 4.050 eV; $E_r \approx$ 0.630 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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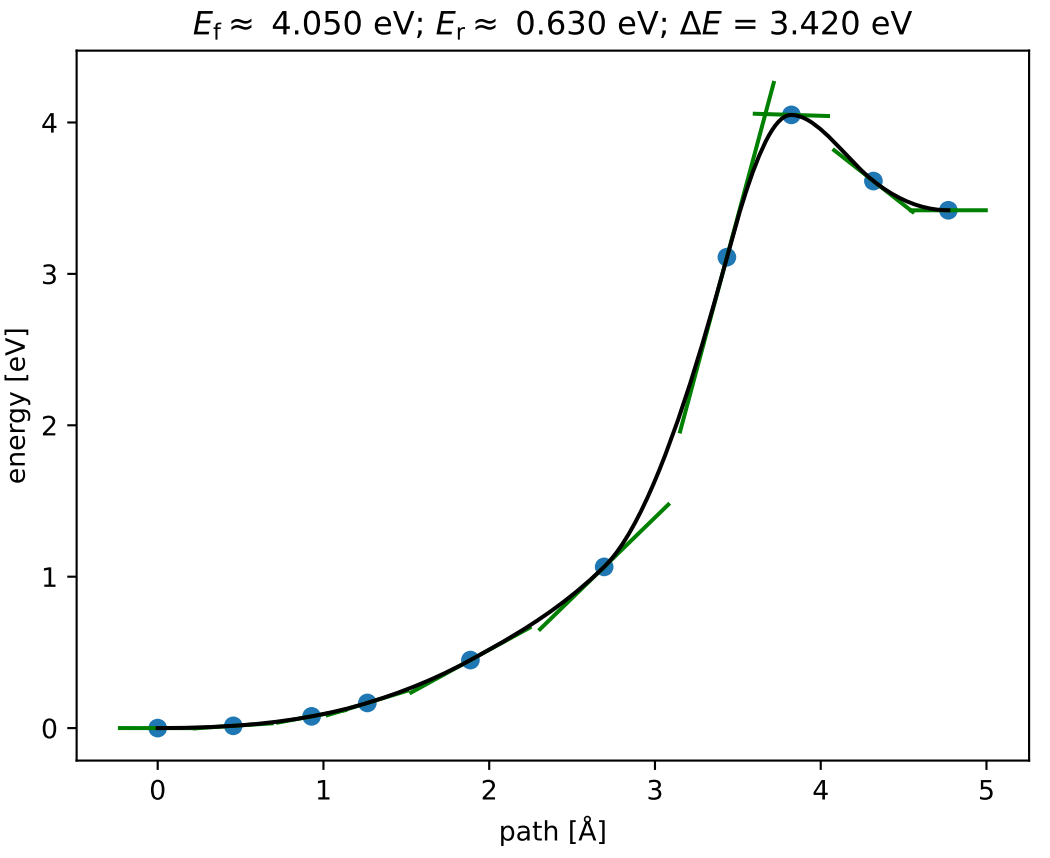
$E_f \approx$ 4.050 eV; $E_r \approx$ 0.630 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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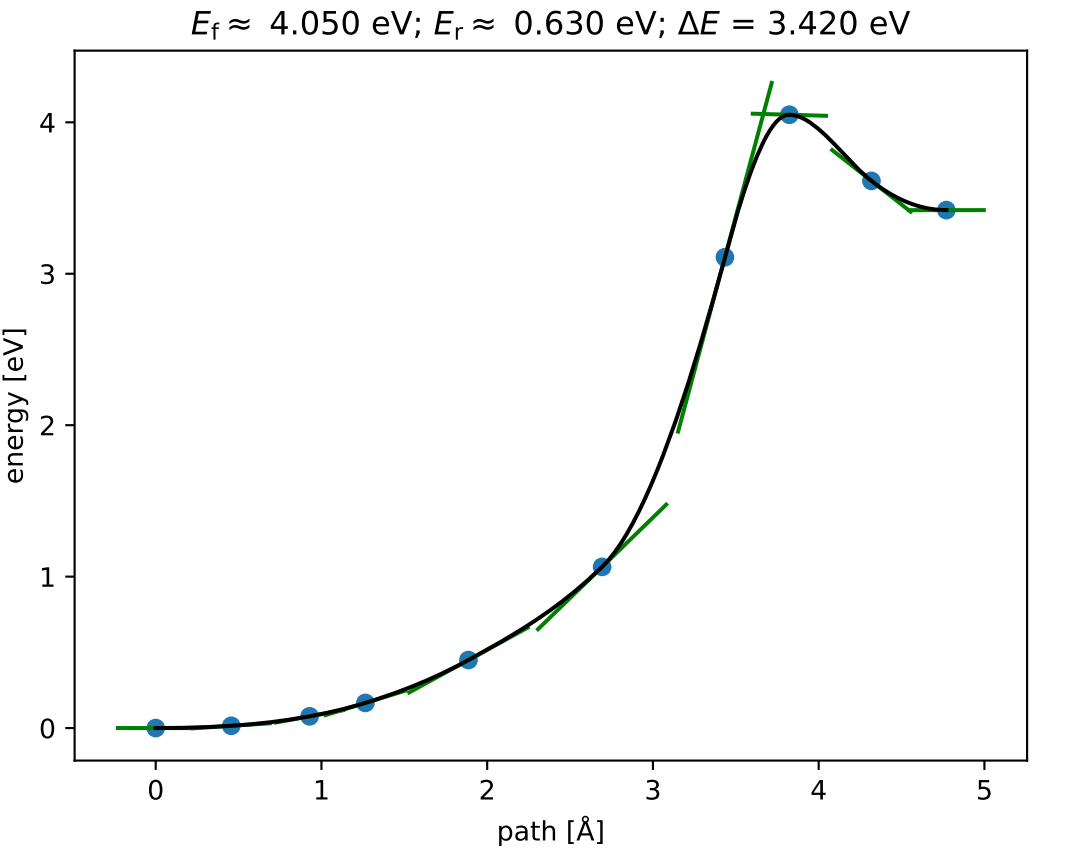
$E_f \approx$ 4.050 eV; $E_r \approx$ 0.630 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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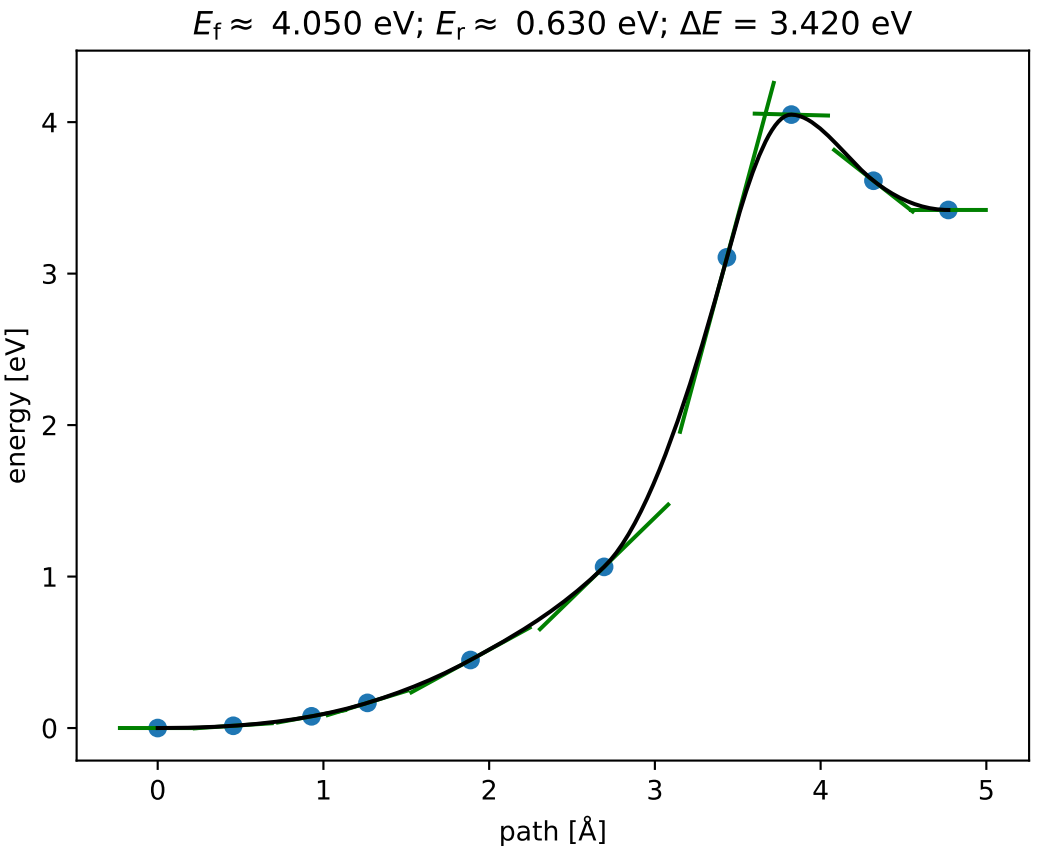
$E_f \approx$ 4.050 eV; $E_r \approx$ 0.630 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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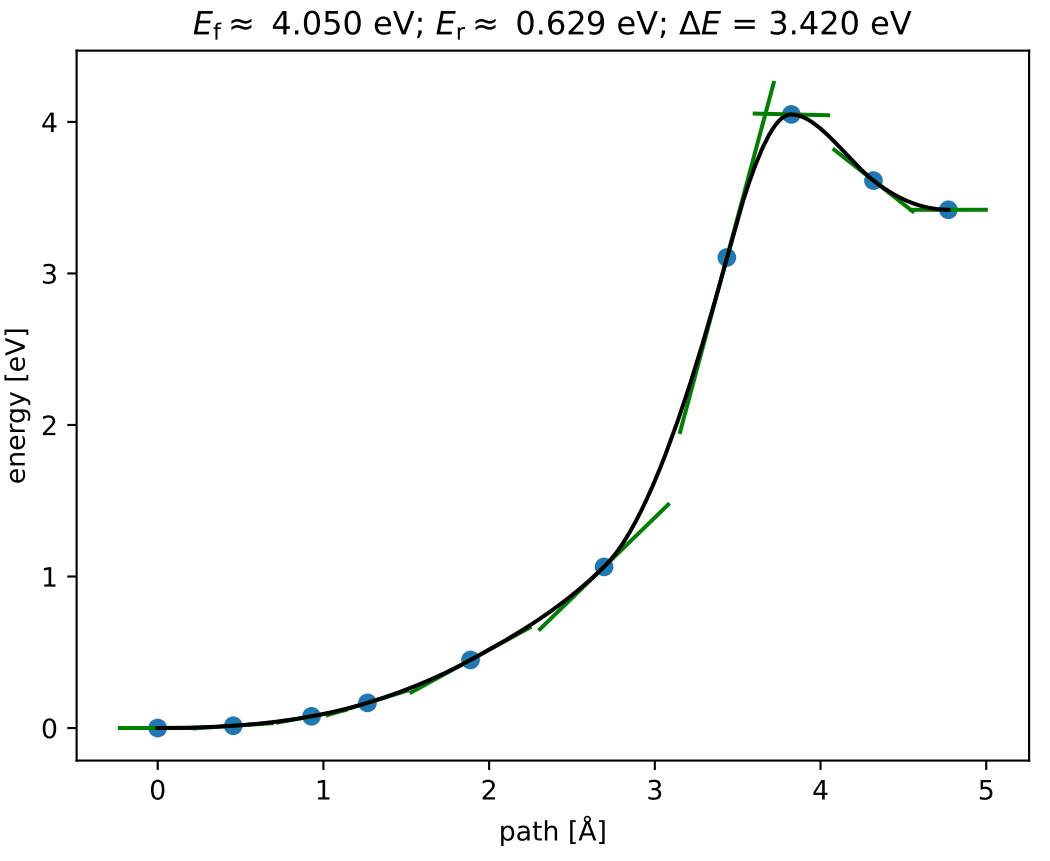
$E_f \approx$ 4.050 eV; $E_r \approx$ 0.629 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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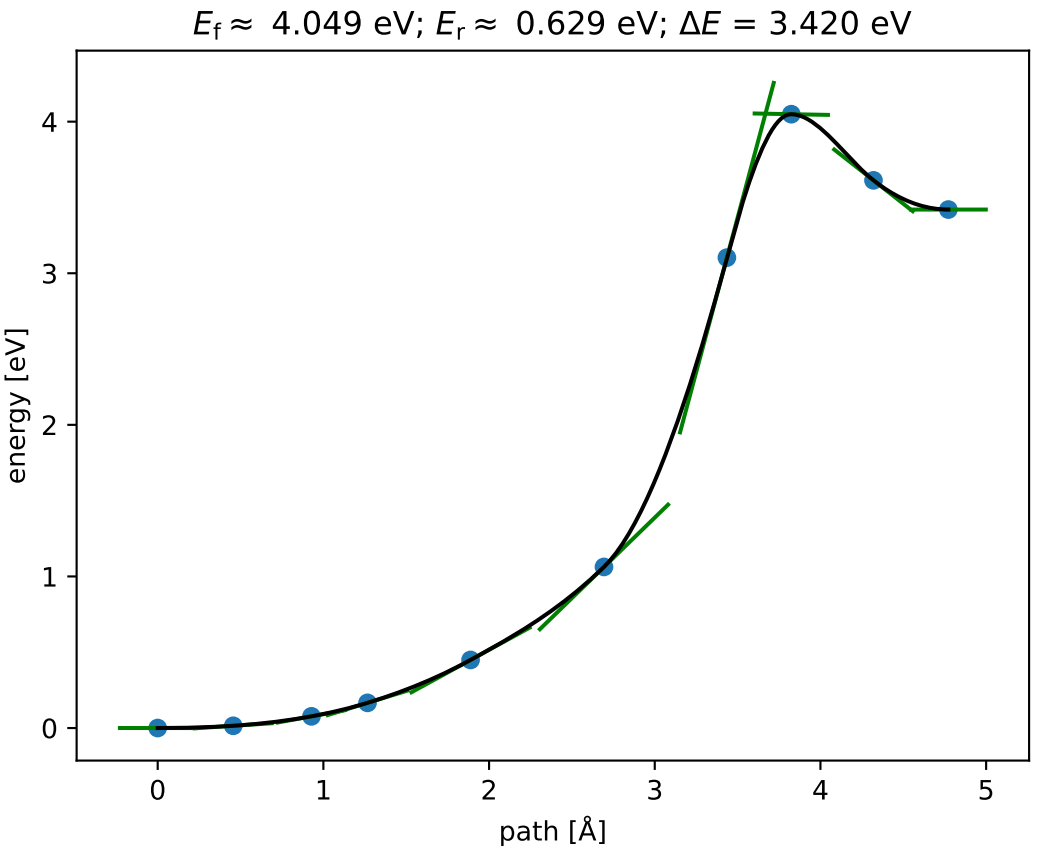
$E_f \approx$ 4.049 eV; $E_r \approx$ 0.629 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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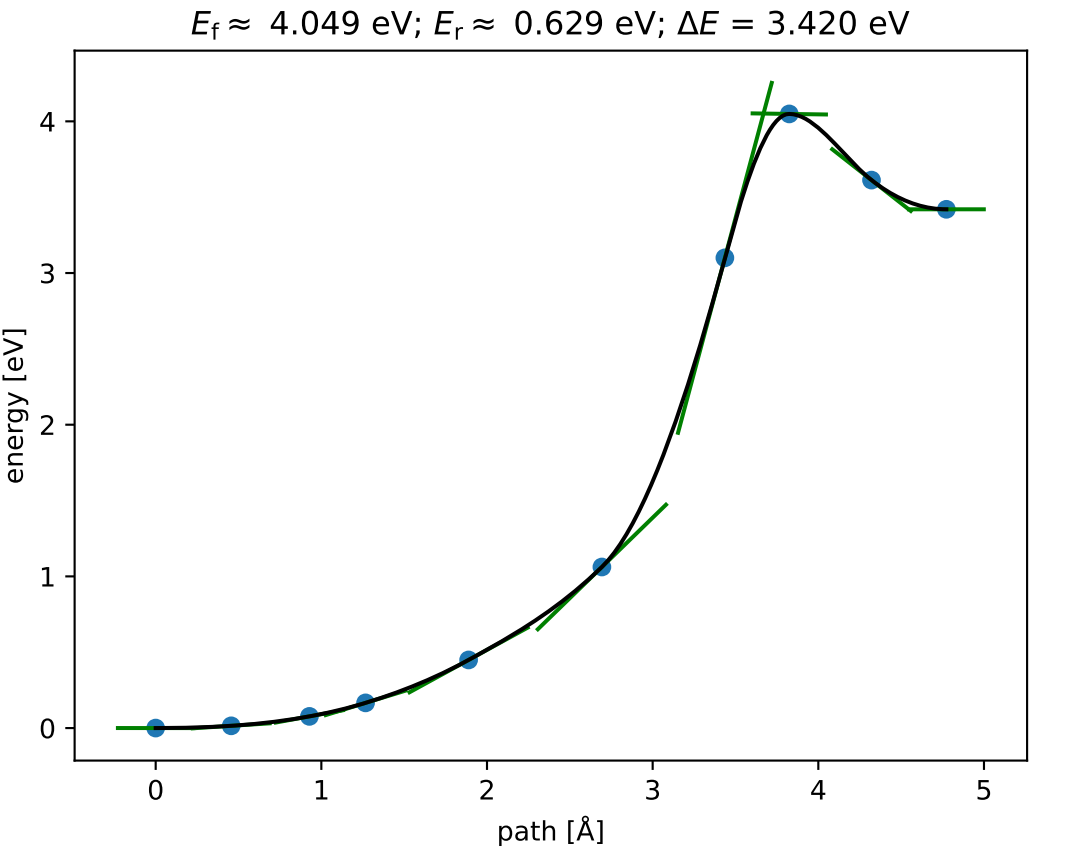
$E_f \approx$ 4.049 eV; $E_r \approx$ 0.629 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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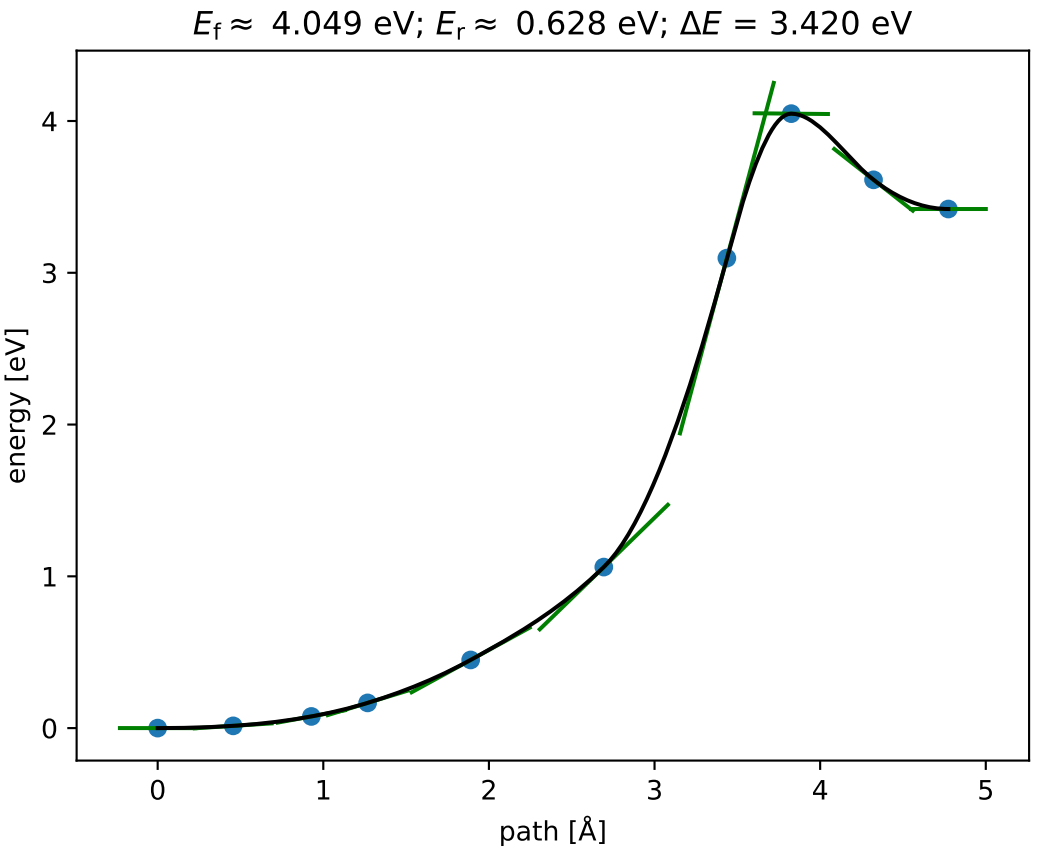
$E_f \approx$ 4.049 eV; $E_r \approx$ 0.628 eV; ΔE = 3.420 eV
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path [Å]
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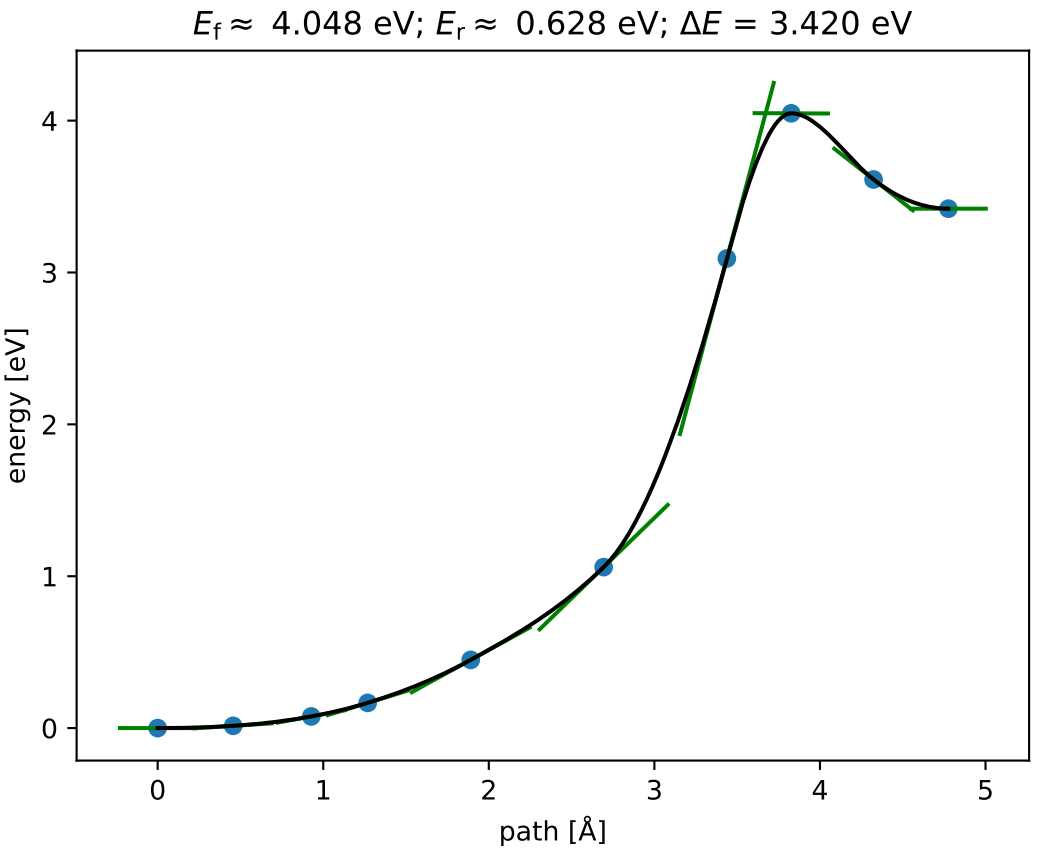
$E_f \approx$ 4.048 eV; $E_r \approx$ 0.628 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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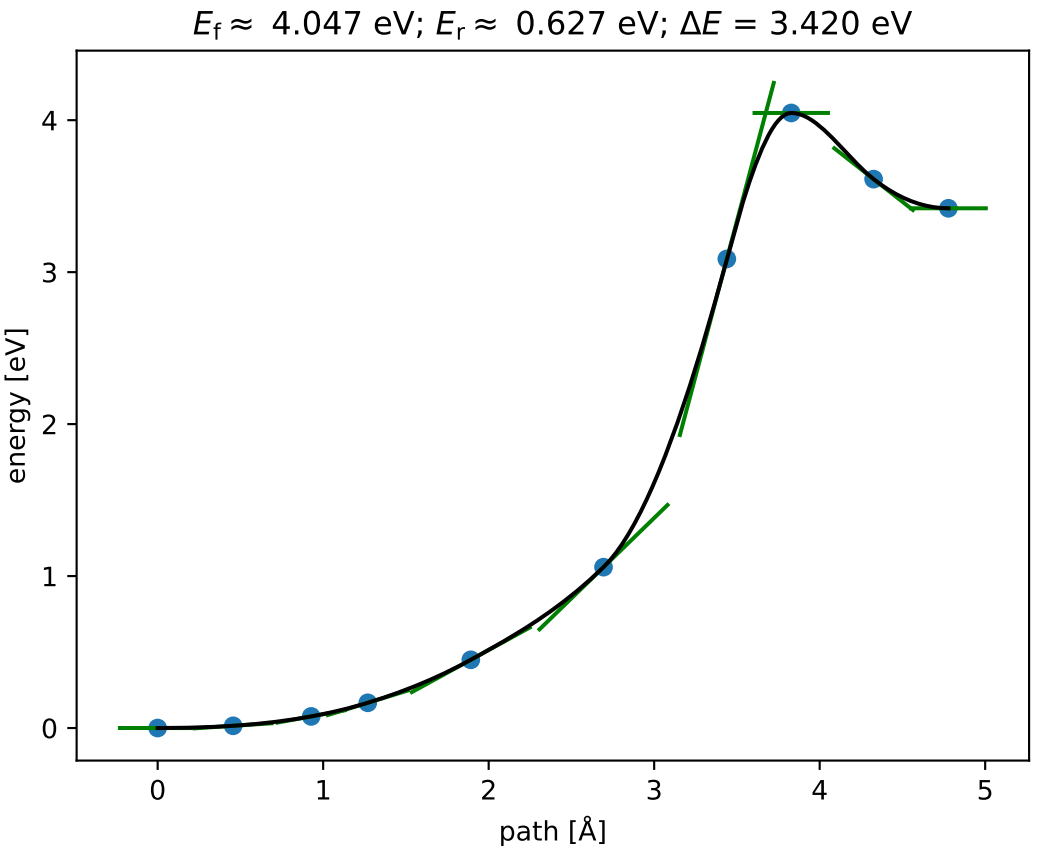
$E_f \approx$ 4.047 eV; $E_r \approx$ 0.627 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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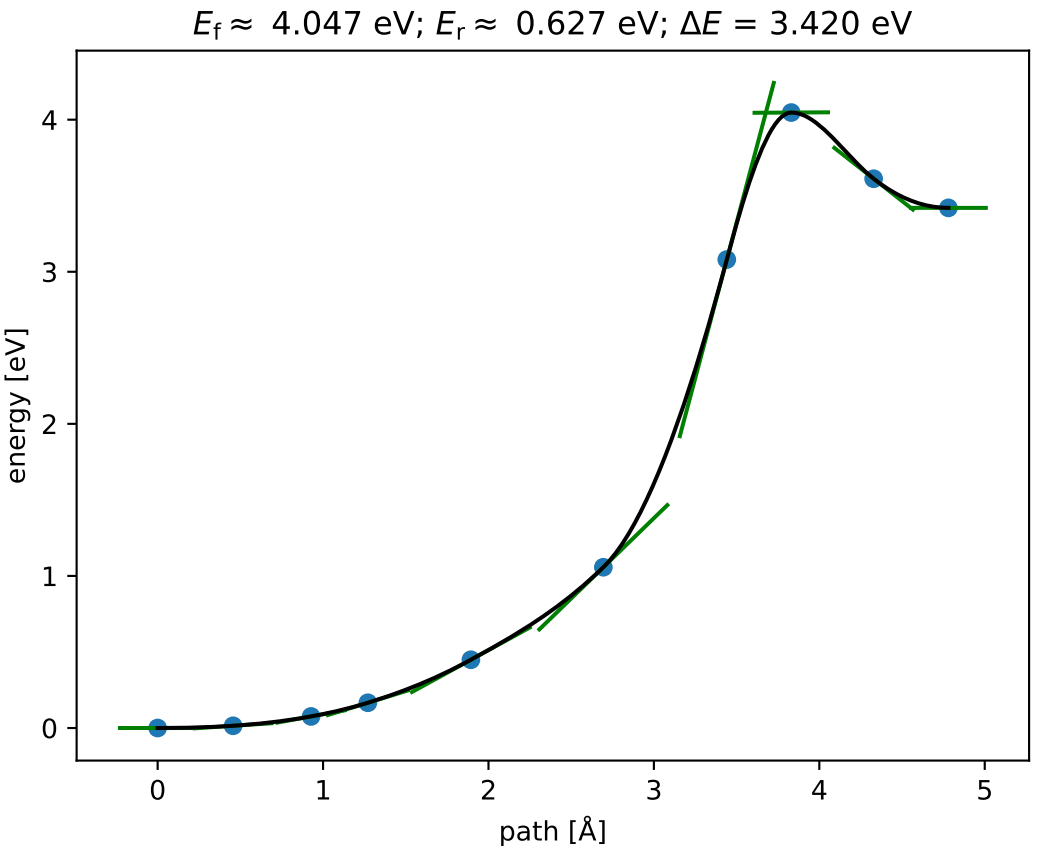
$E_f \approx$ 4.047 eV; $E_r \approx$ 0.627 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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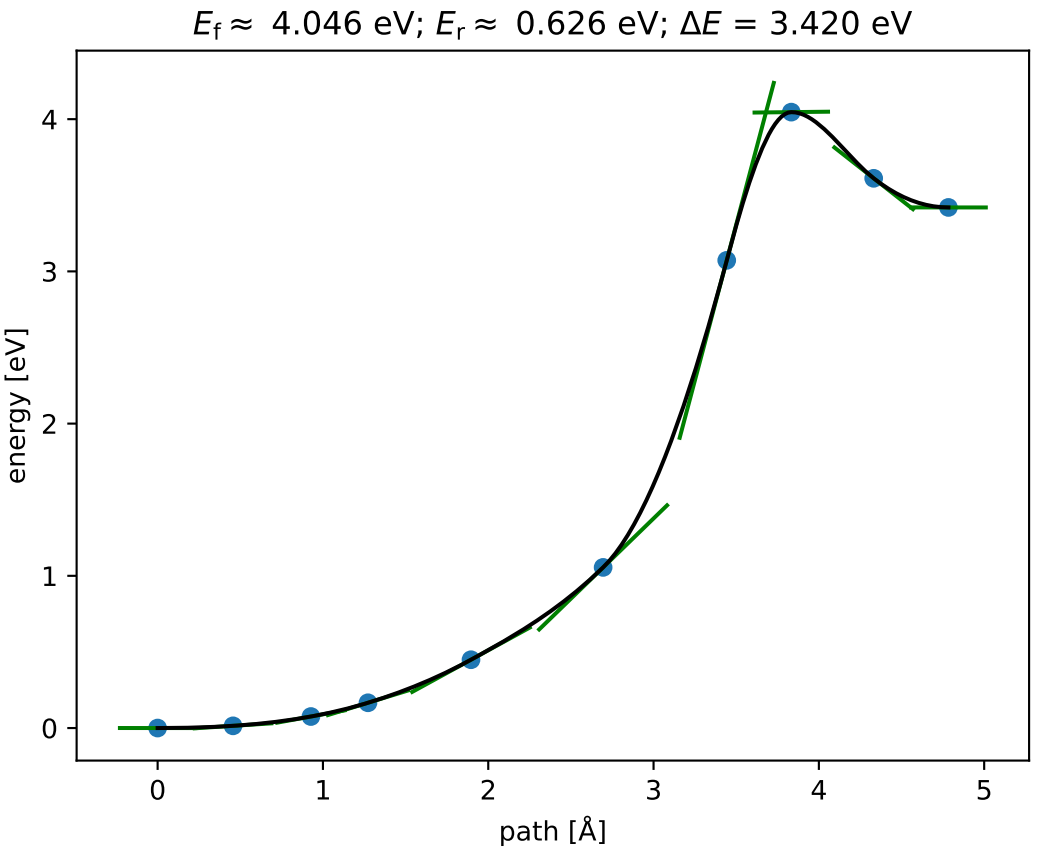
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path [Å]
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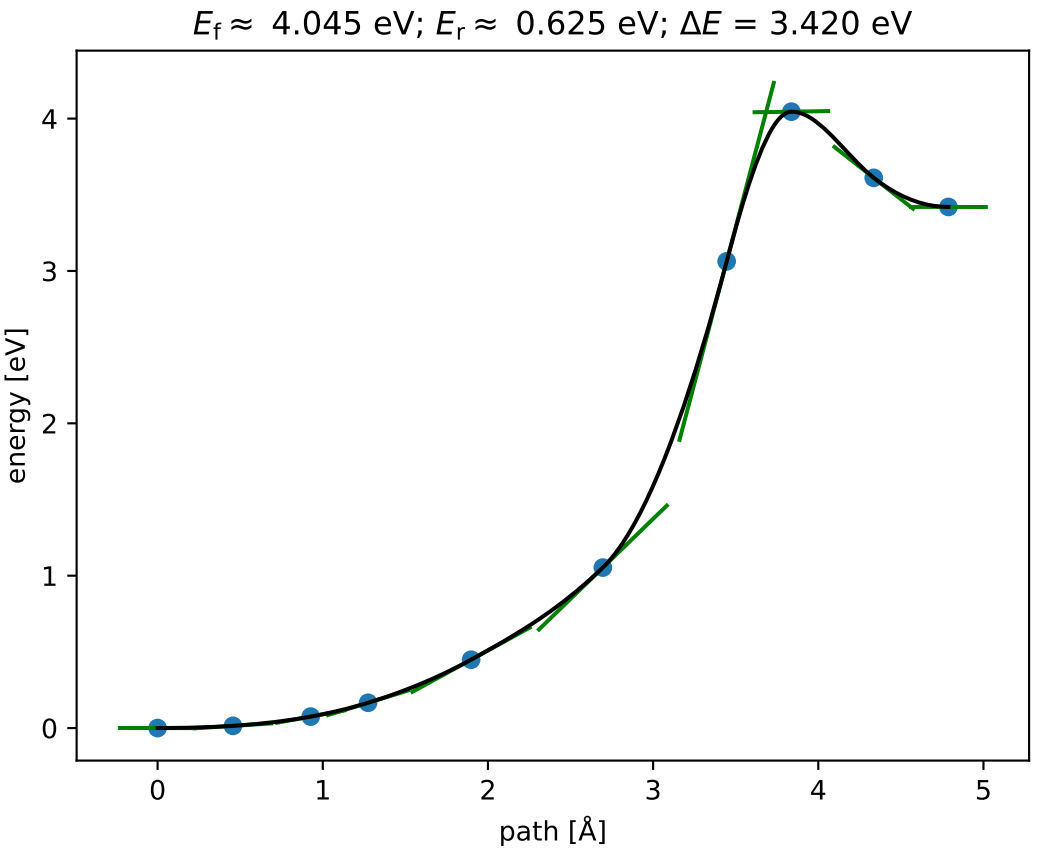
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energy [eV]
path [Å]
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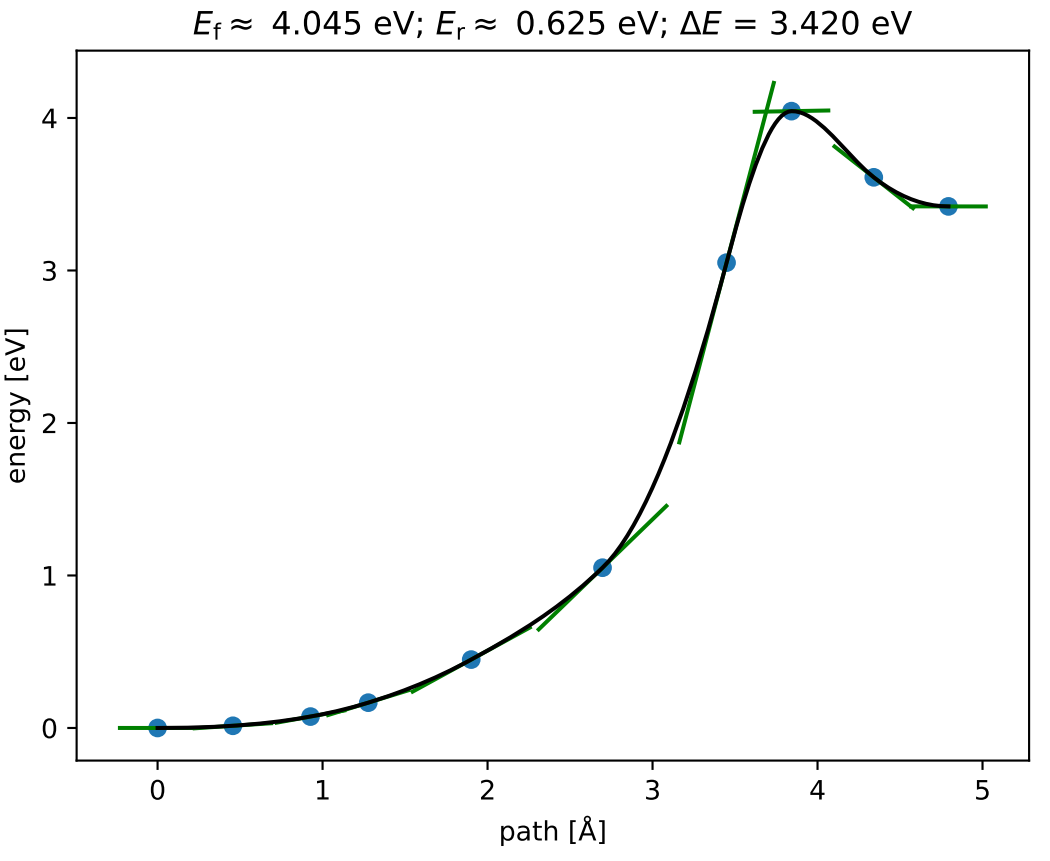
$E_f \approx$ 4.045 eV; $E_r \approx$ 0.625 eV; ΔE = 3.420 eV
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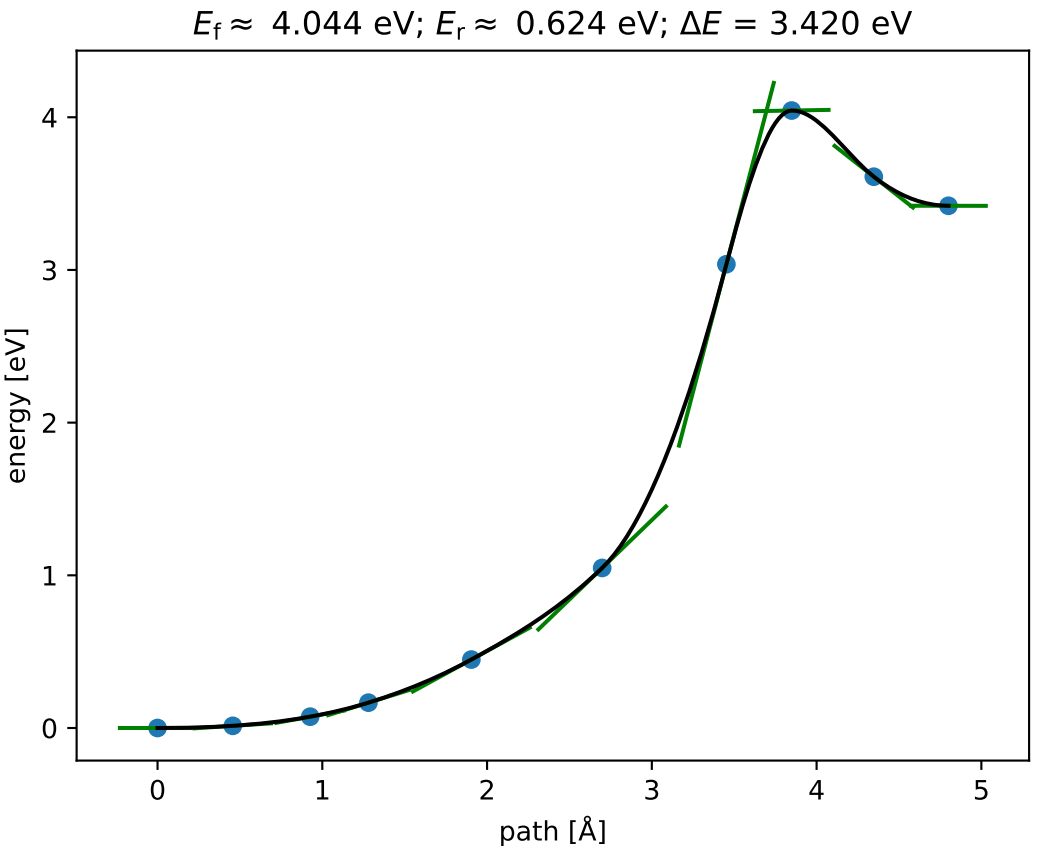
$E_f \approx$ 4.044 eV; $E_r \approx$ 0.624 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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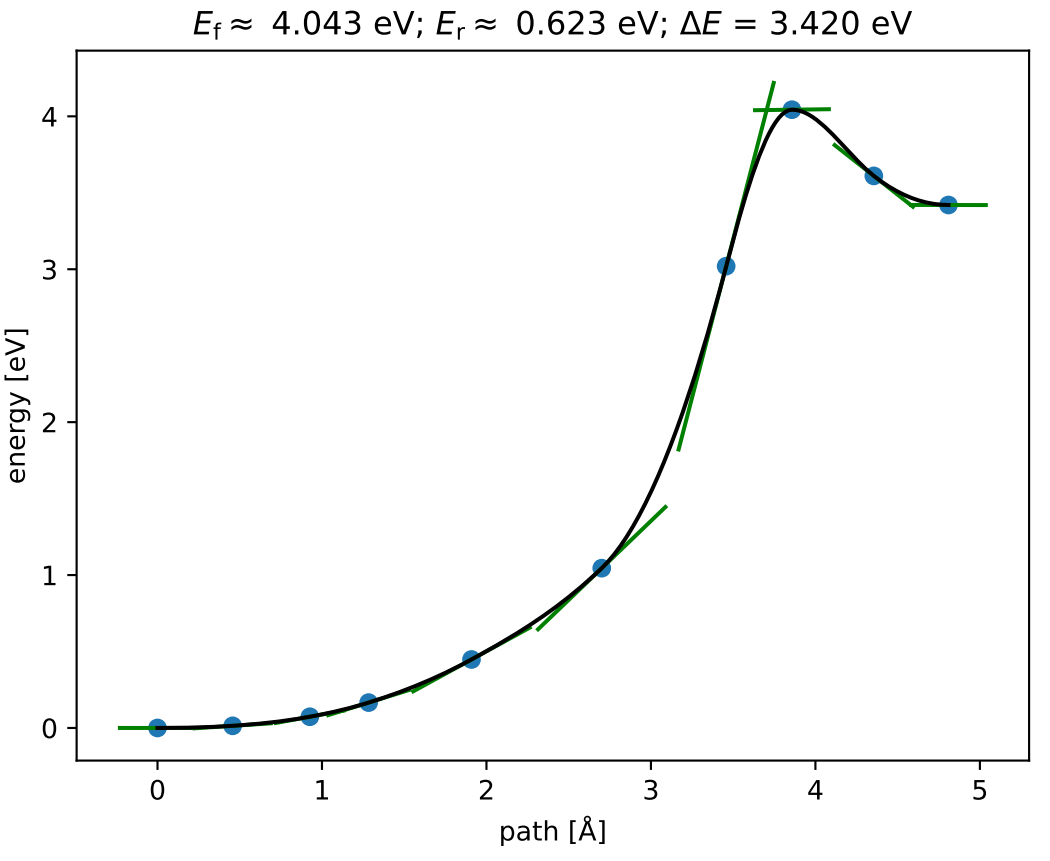
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path [Å]
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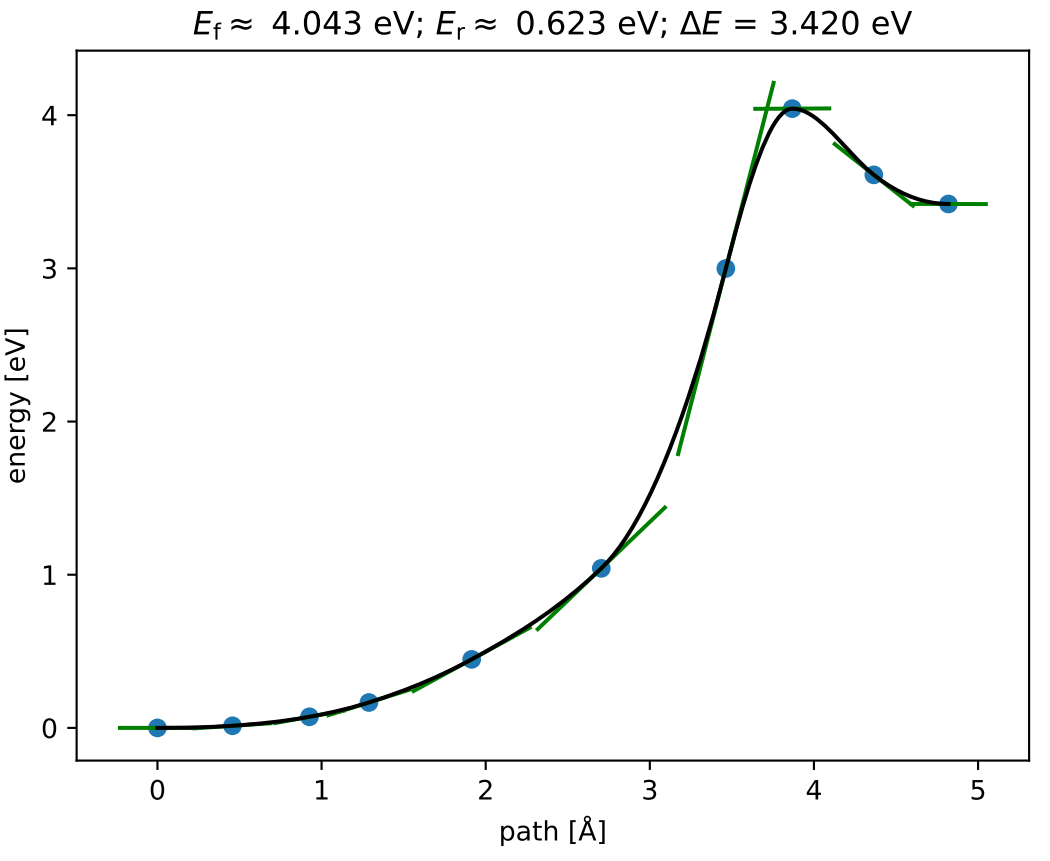
$E_f \approx$ 4.043 eV; $E_r \approx$ 0.623 eV; ΔE = 3.420 eV
energy [eV]
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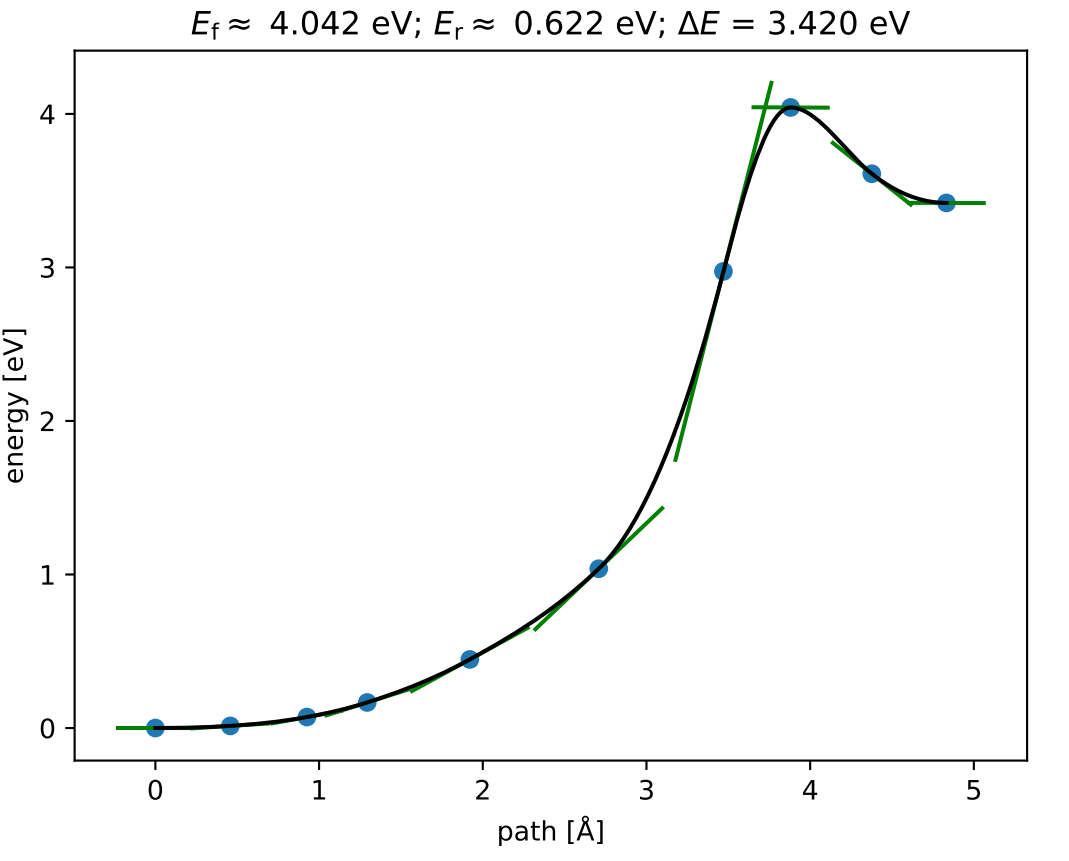
$E_f \approx$ 4.042 eV; $E_r \approx$ 0.622 eV; ΔE = 3.420 eV
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path [Å]
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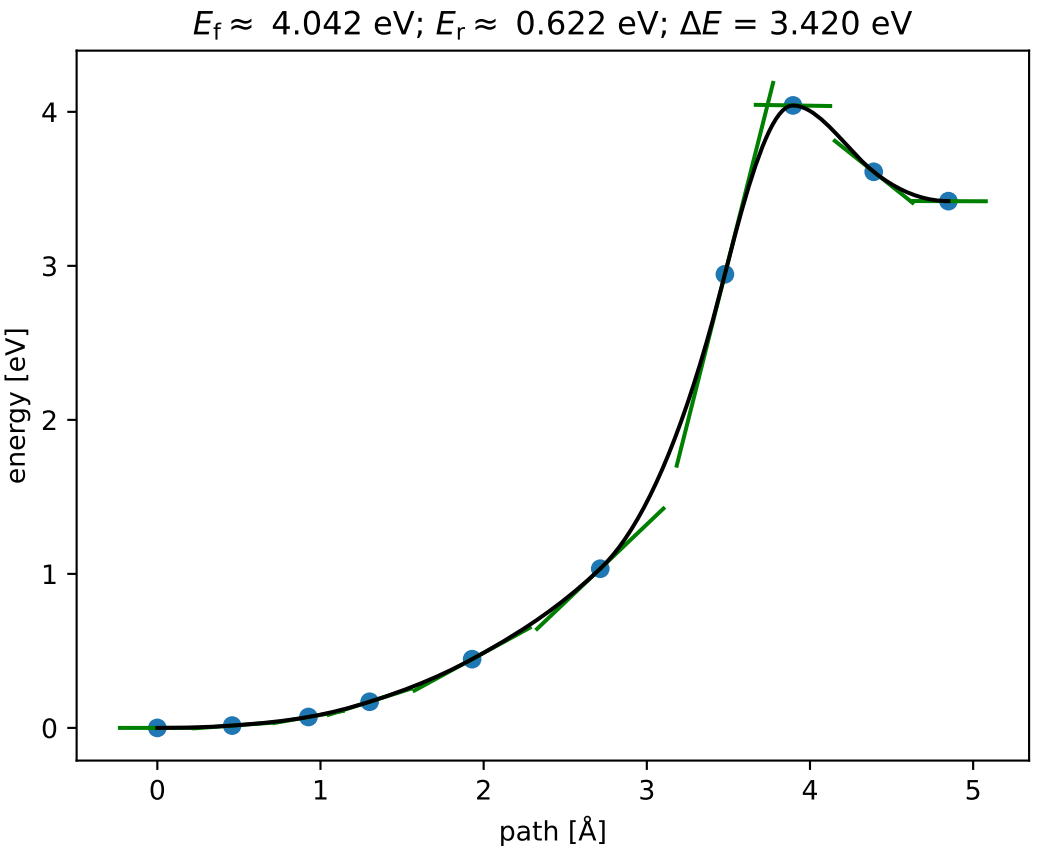
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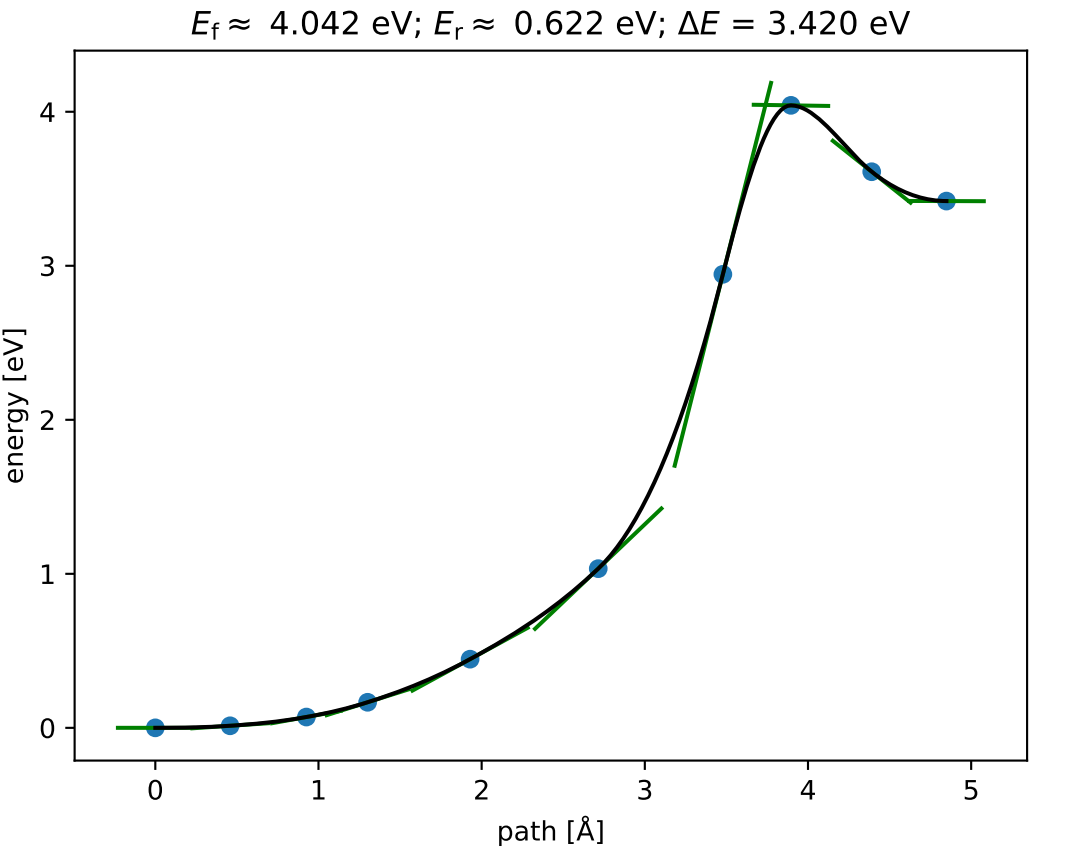
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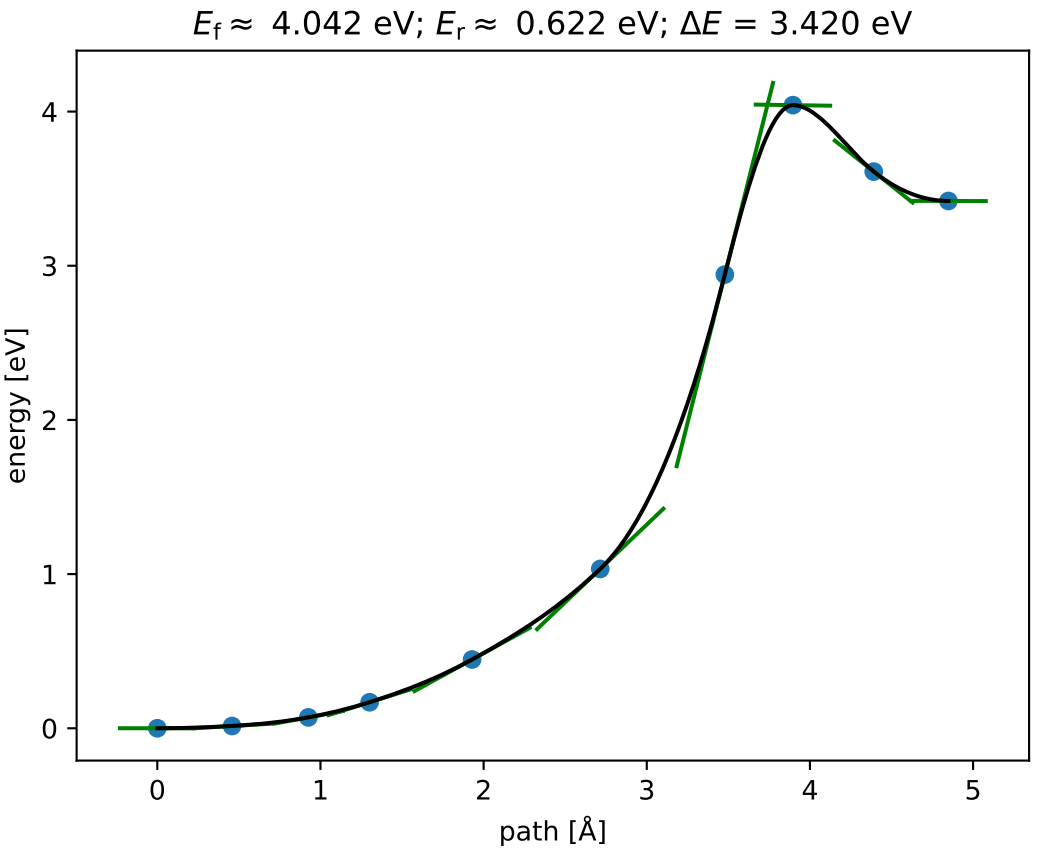
$E_f \approx$ 4.042 eV; $E_r \approx$ 0.622 eV; ΔE = 3.420 eV
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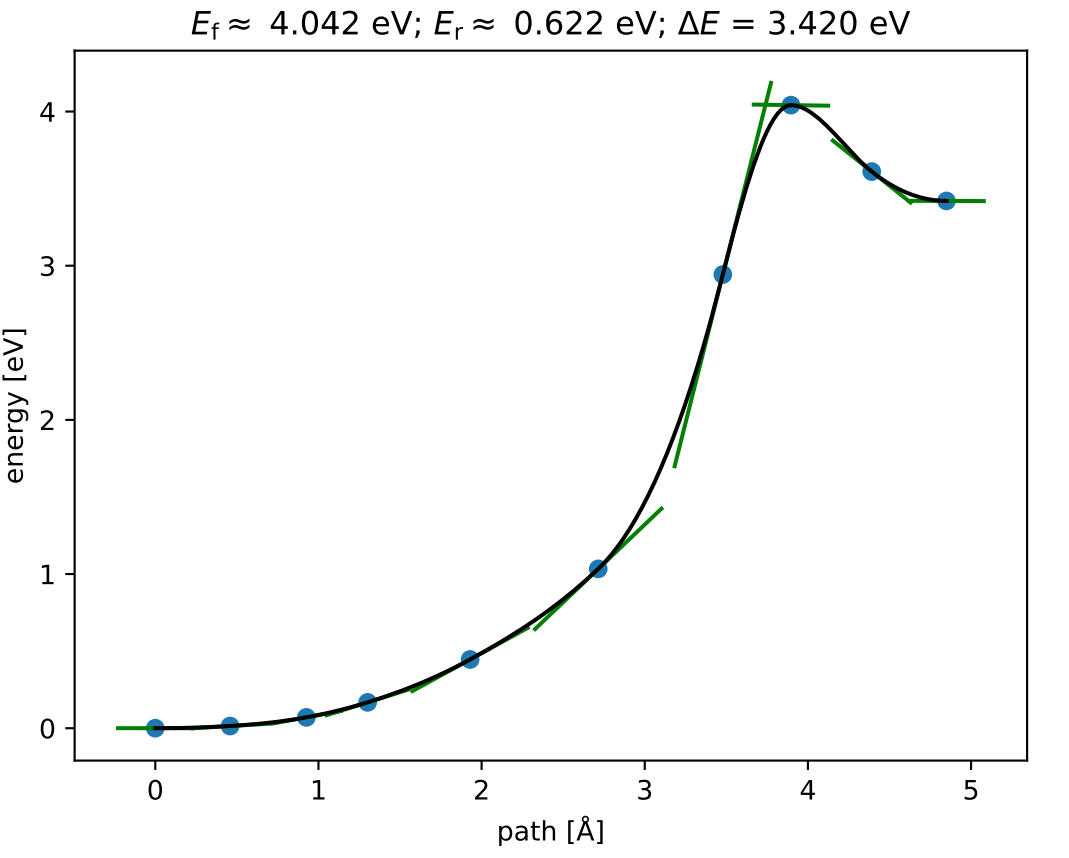
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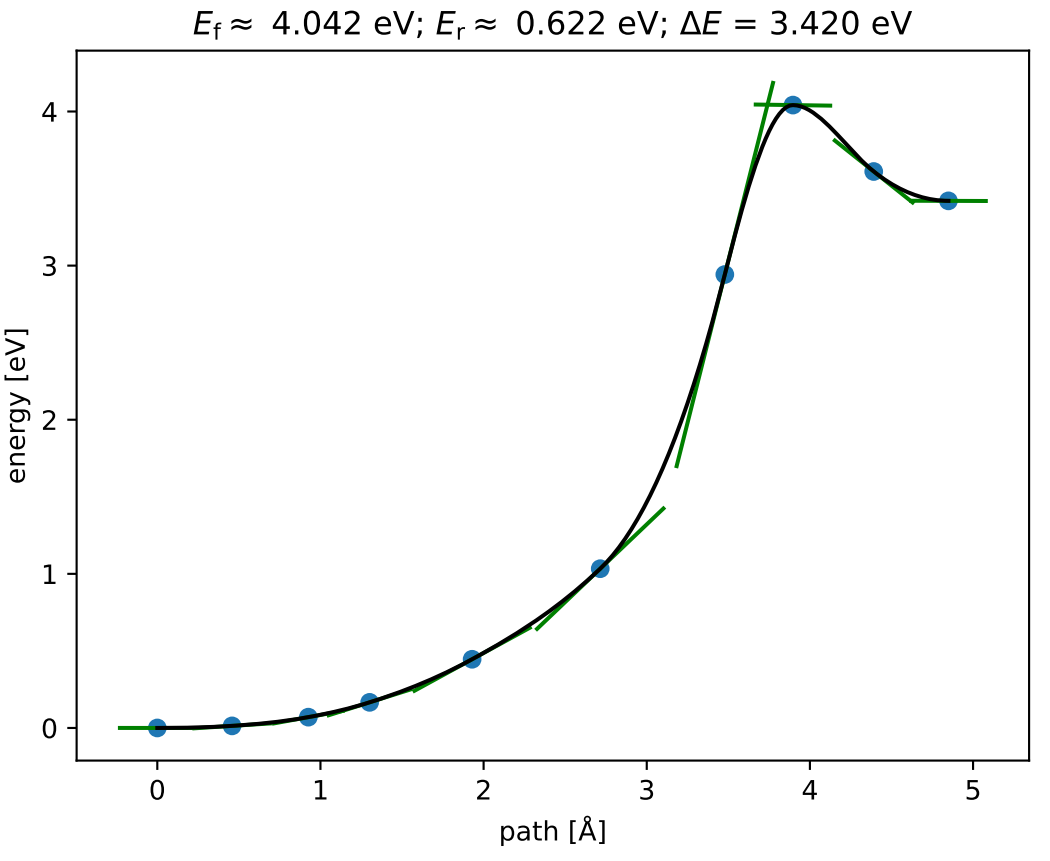
$E_f \approx$ 4.042 eV; $E_r \approx$ 0.622 eV; ΔE = 3.420 eV
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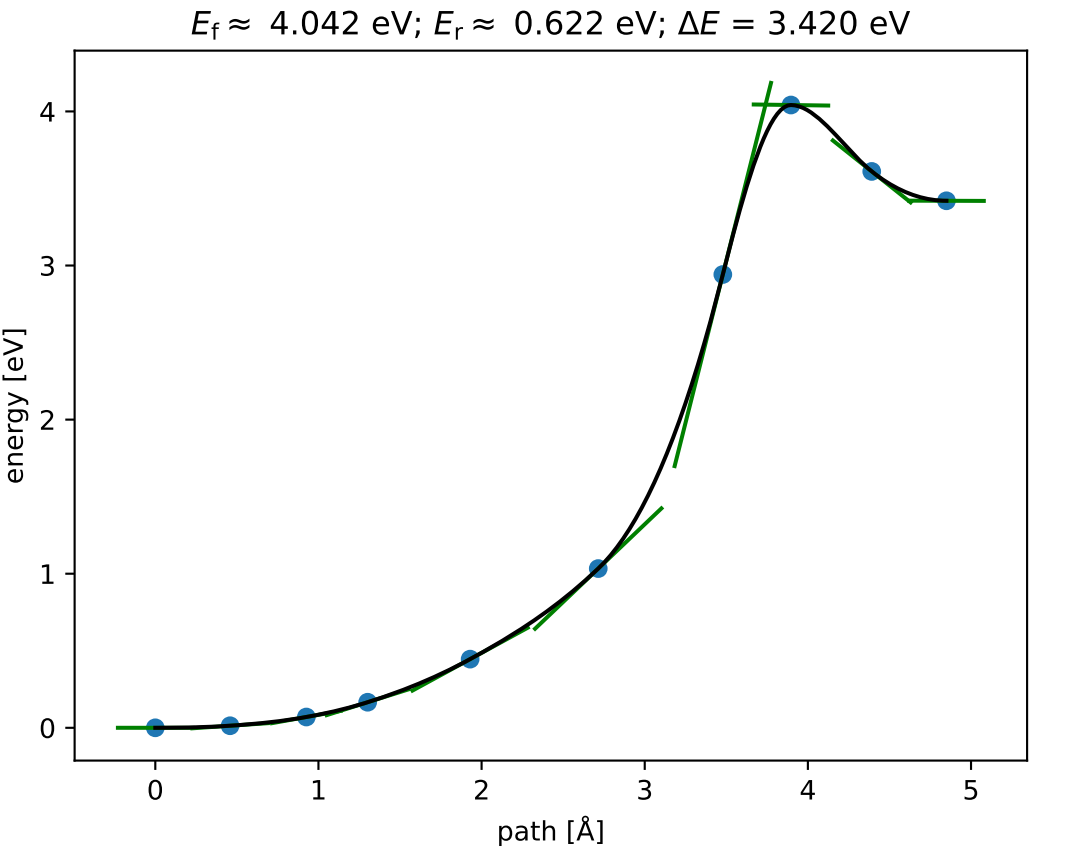
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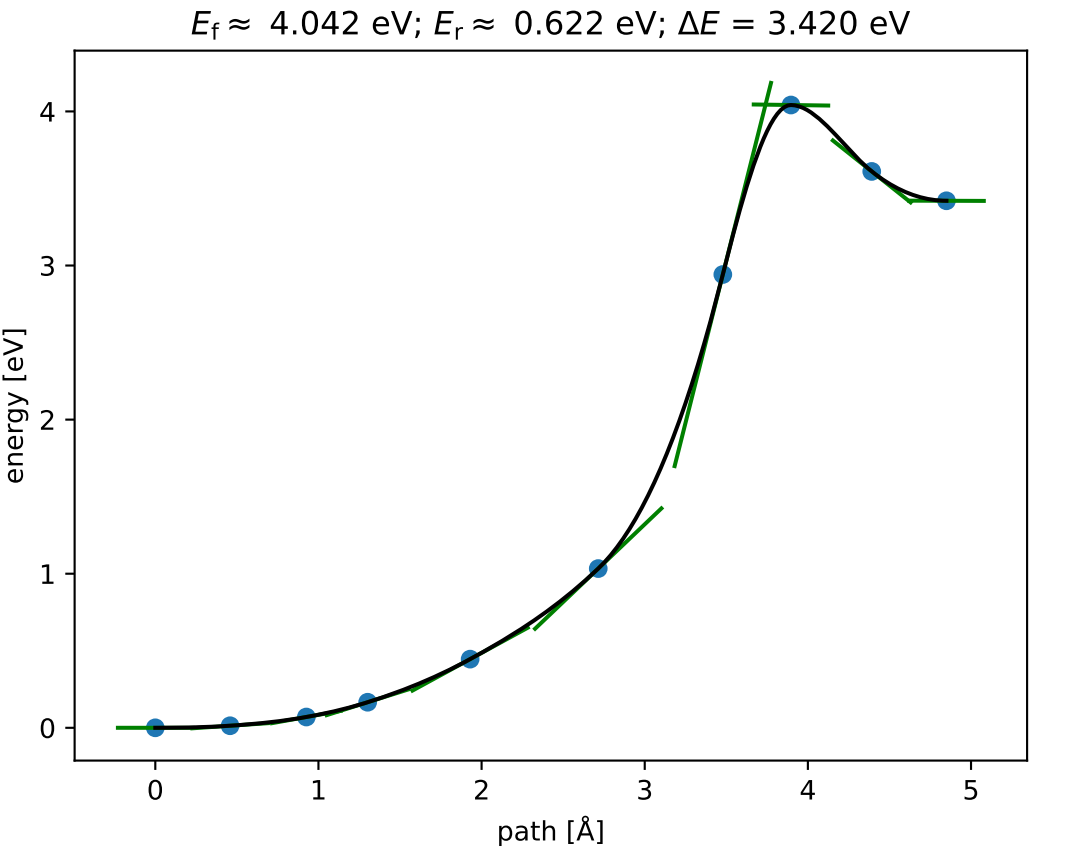
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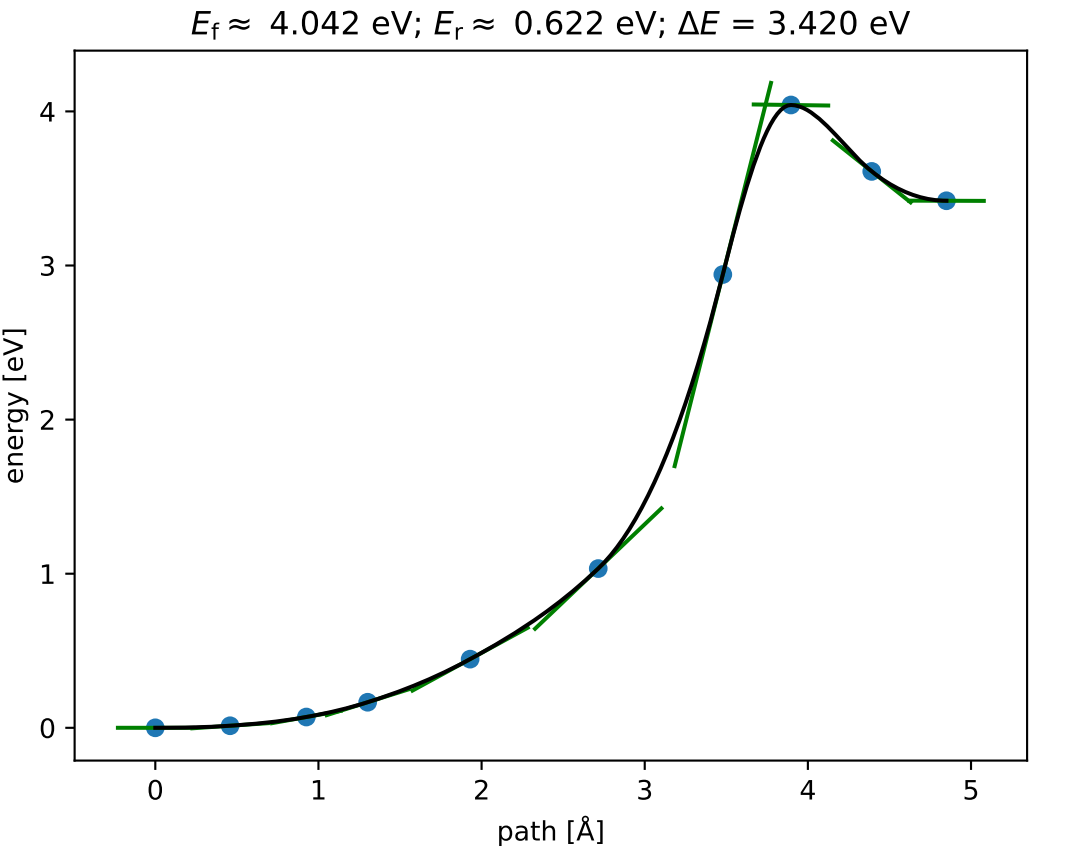
$E_f \approx$ 4.042 eV; $E_r \approx$ 0.622 eV; ΔE = 3.420 eV
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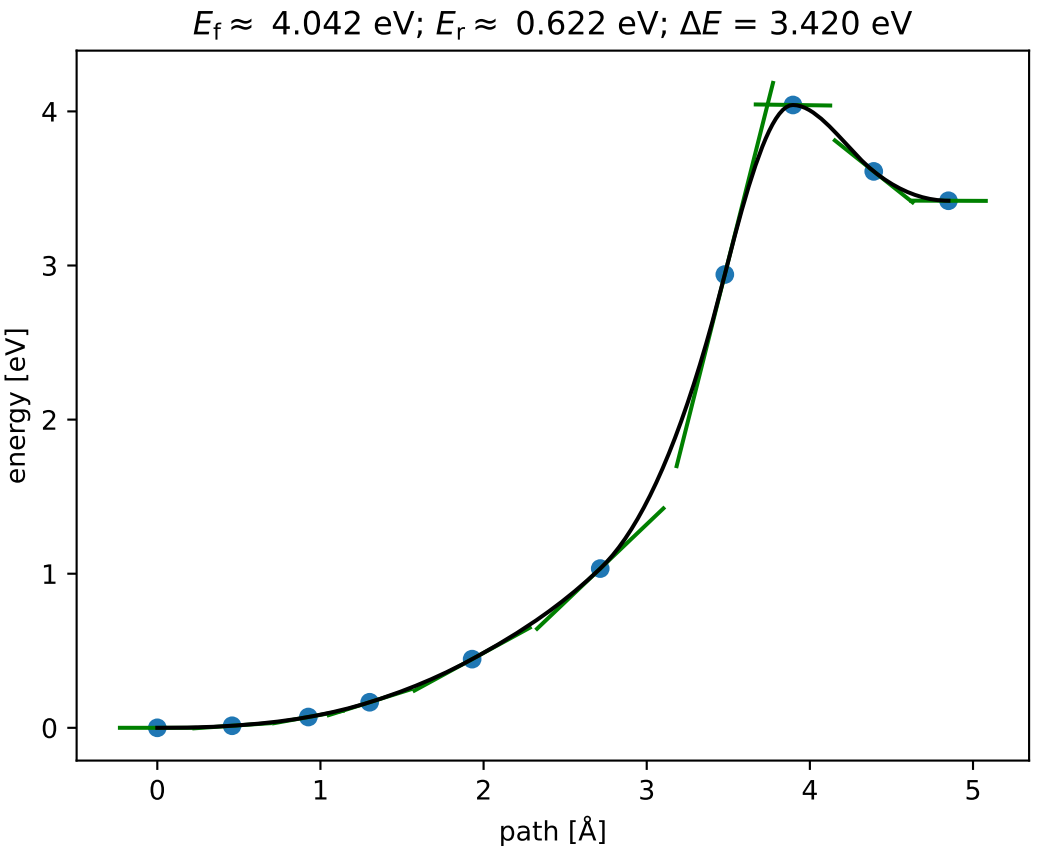
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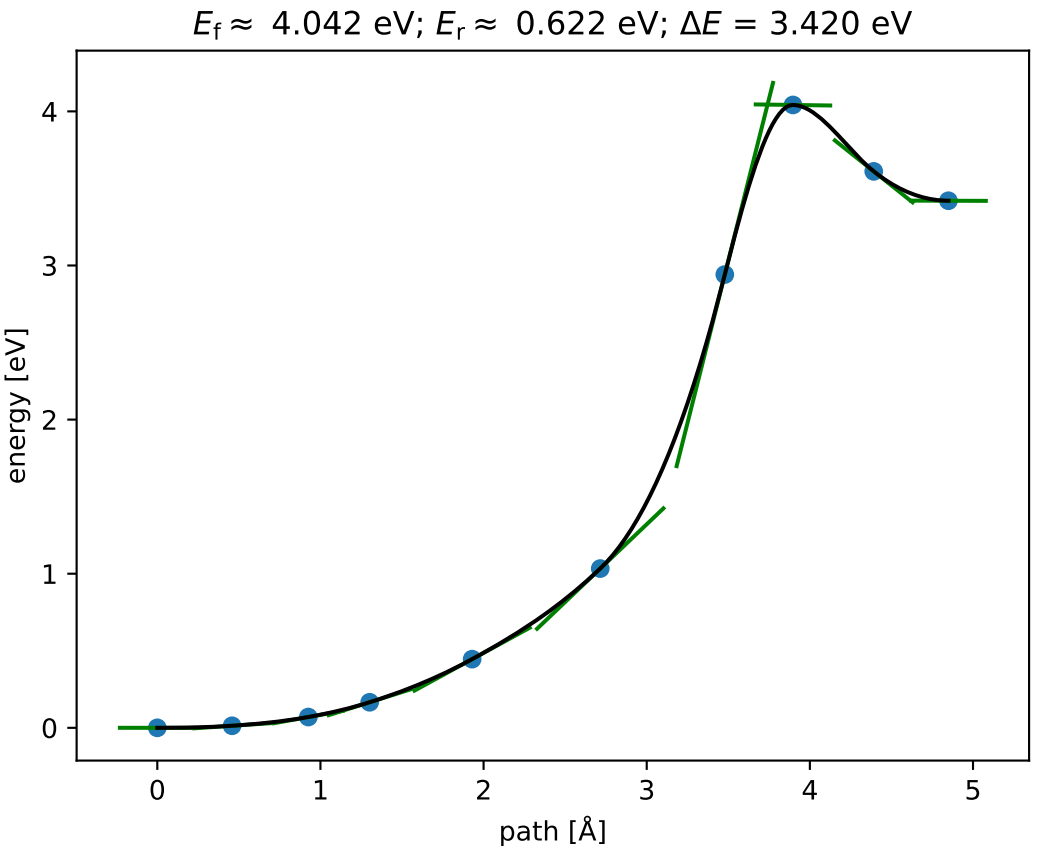
$E_f \approx$ 4.042 eV; $E_r \approx$ 0.622 eV; ΔE = 3.420 eV
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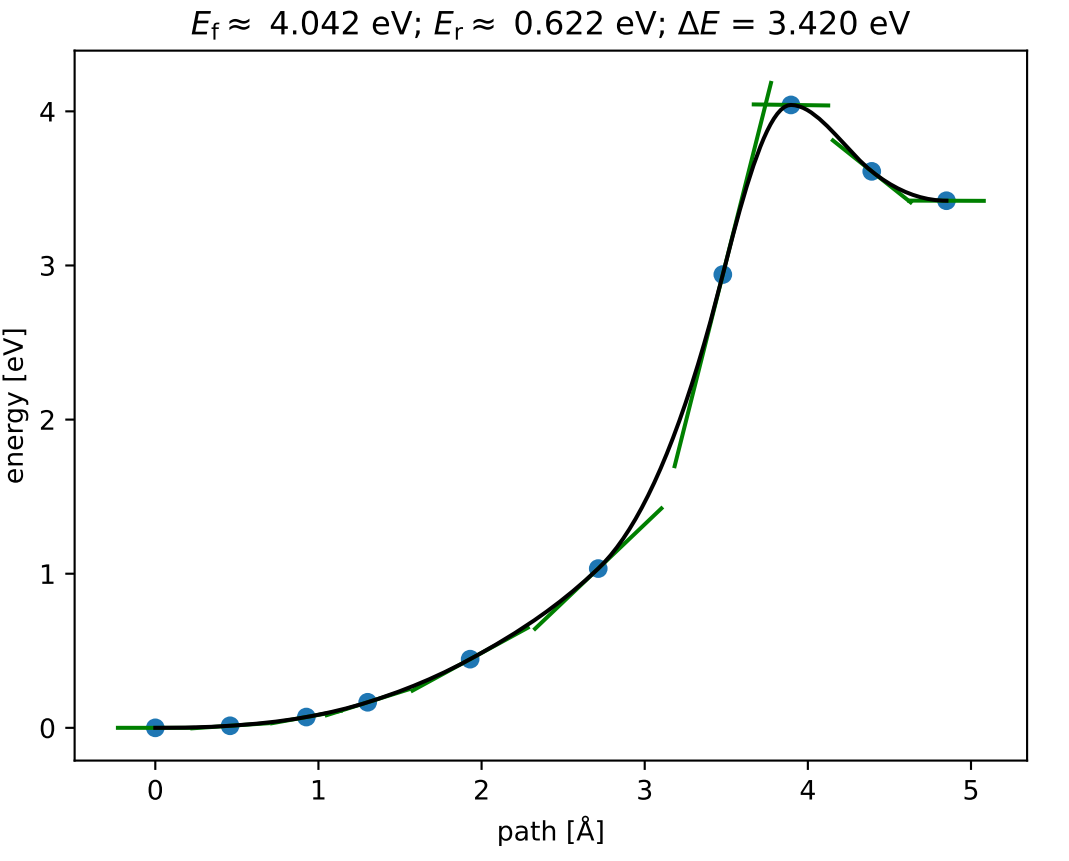
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path [Å]
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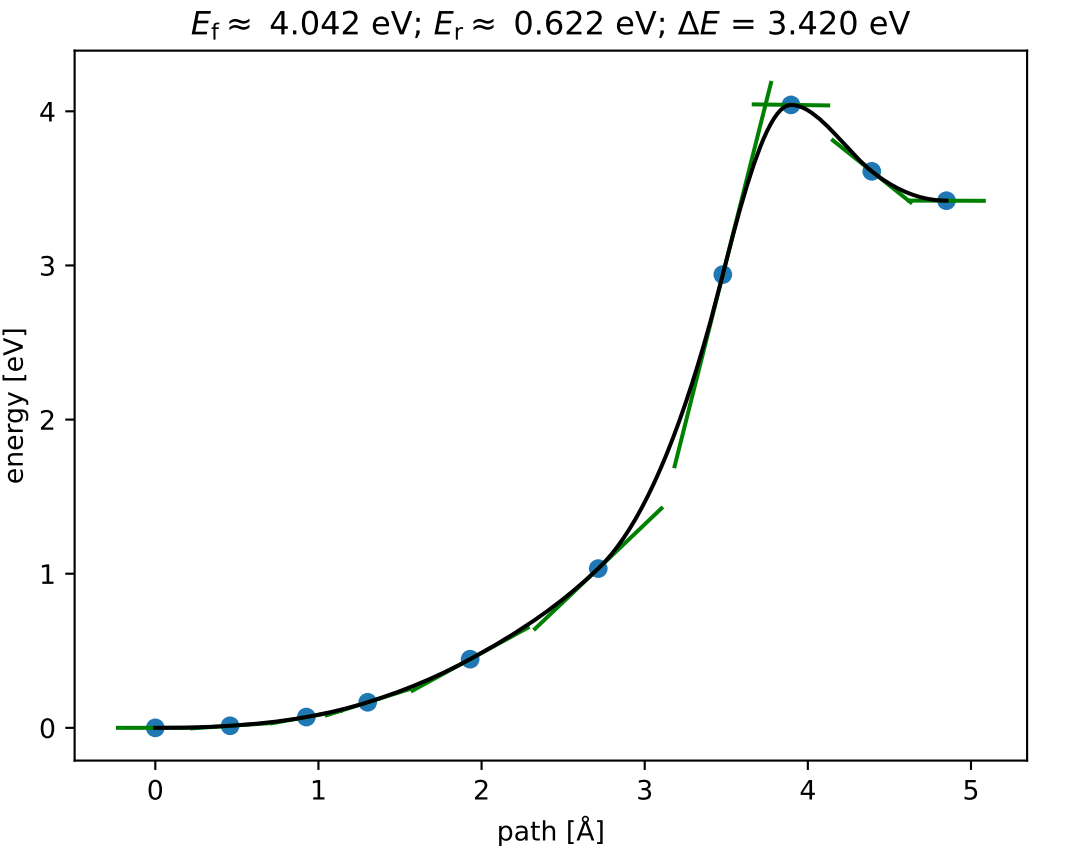
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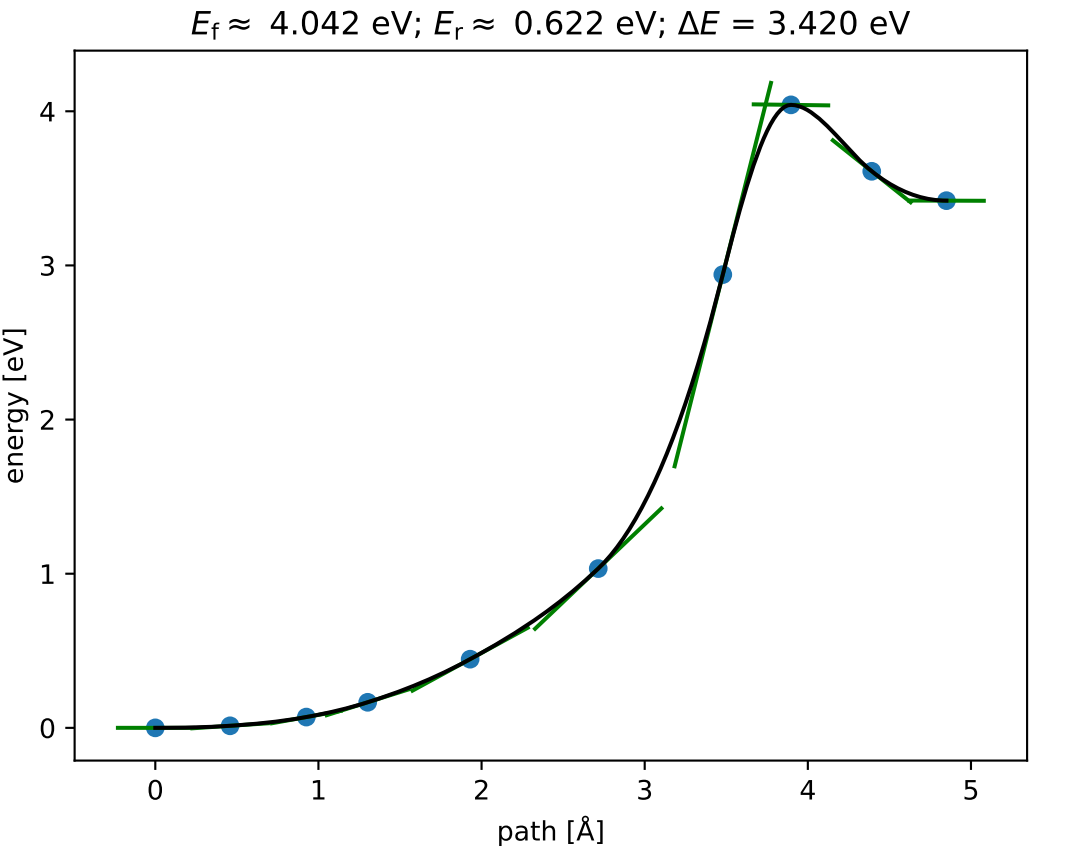
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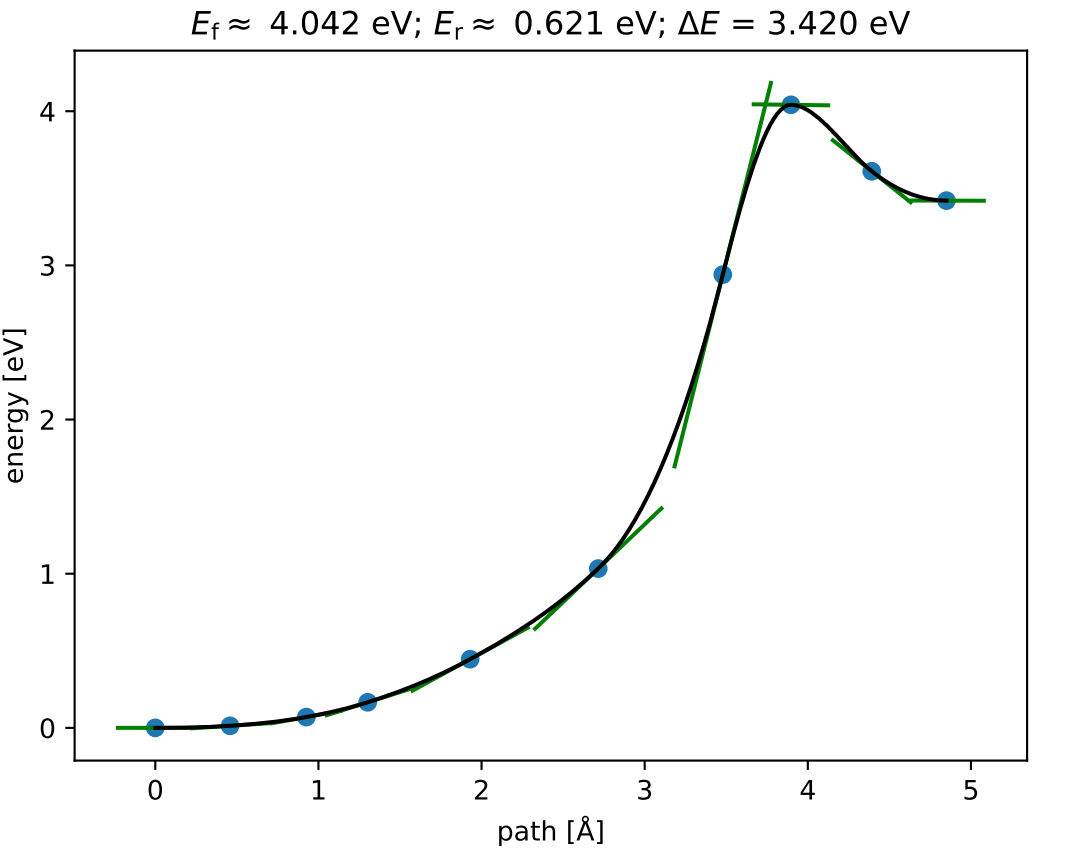
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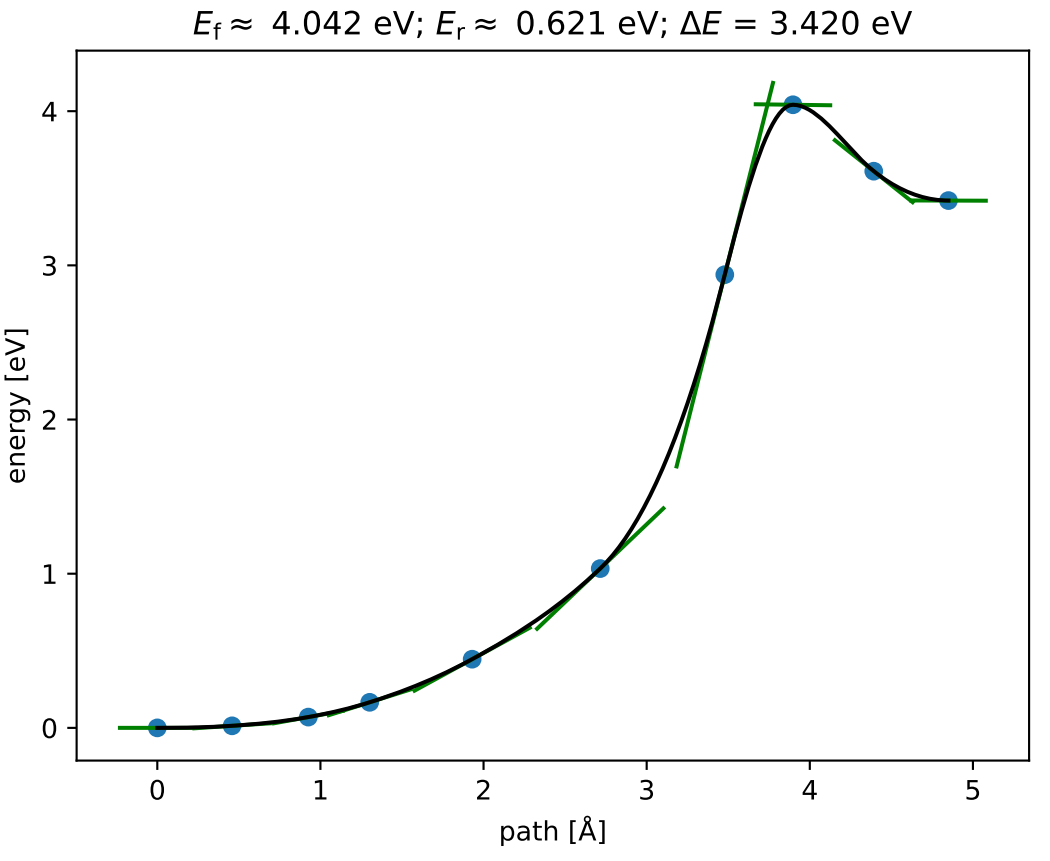
$E_f \approx$ 4.042 eV; $E_r \approx$ 0.621 eV; ΔE = 3.420 eV
energy [eV]
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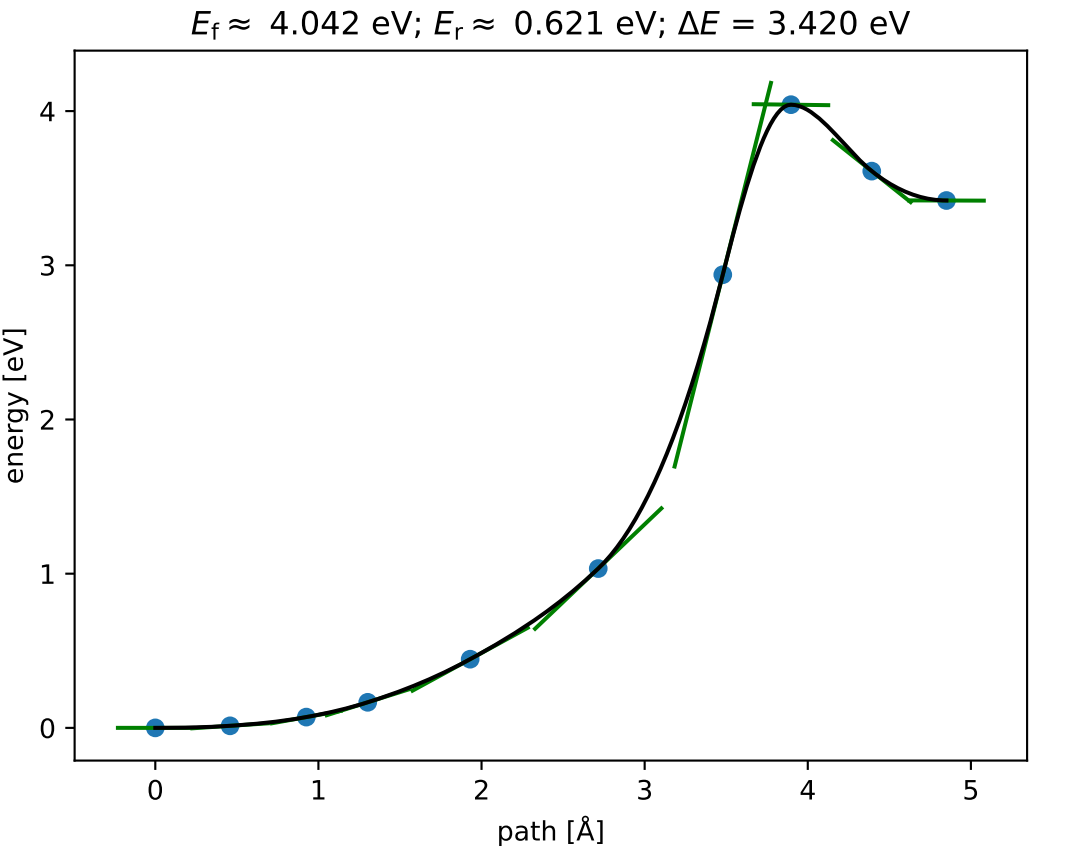
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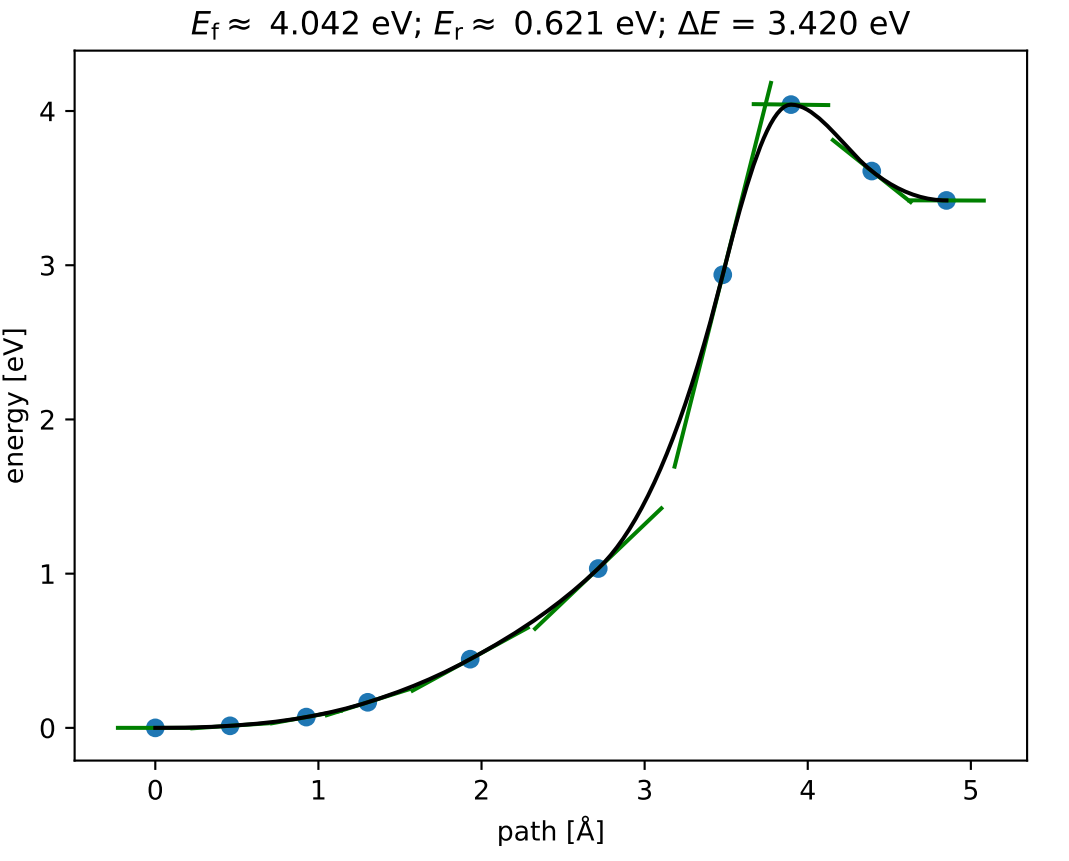
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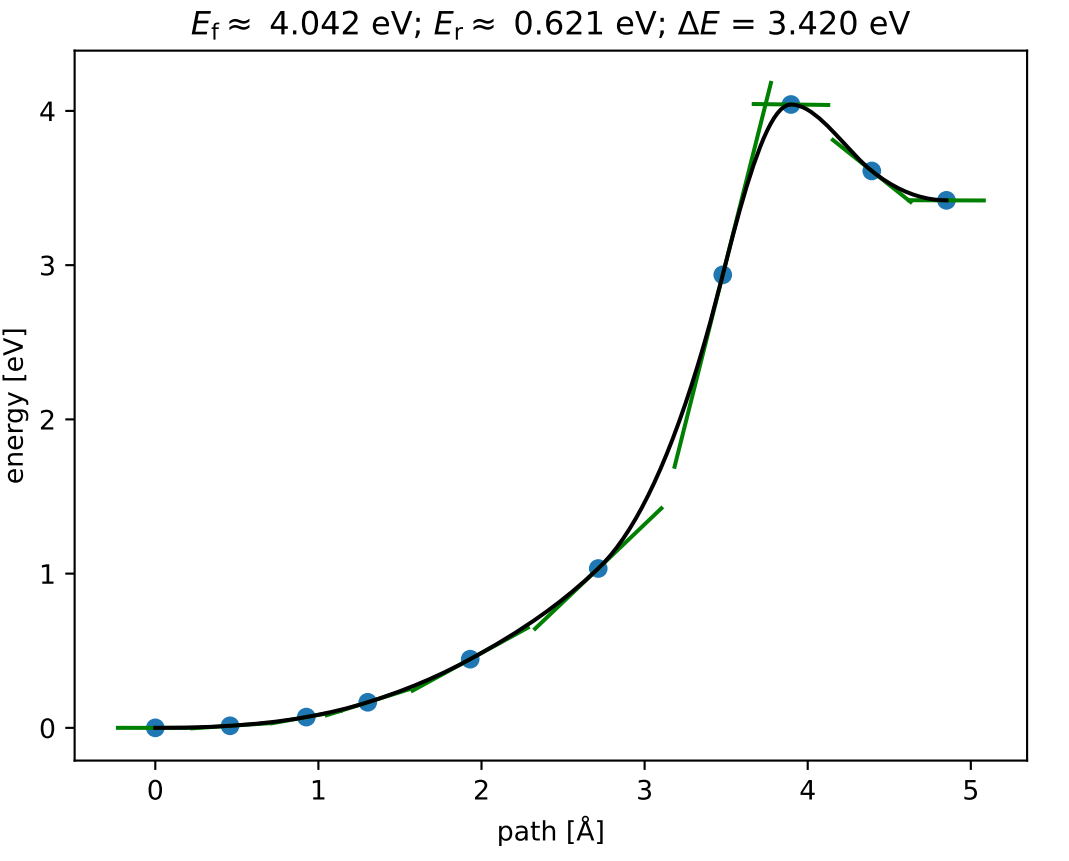
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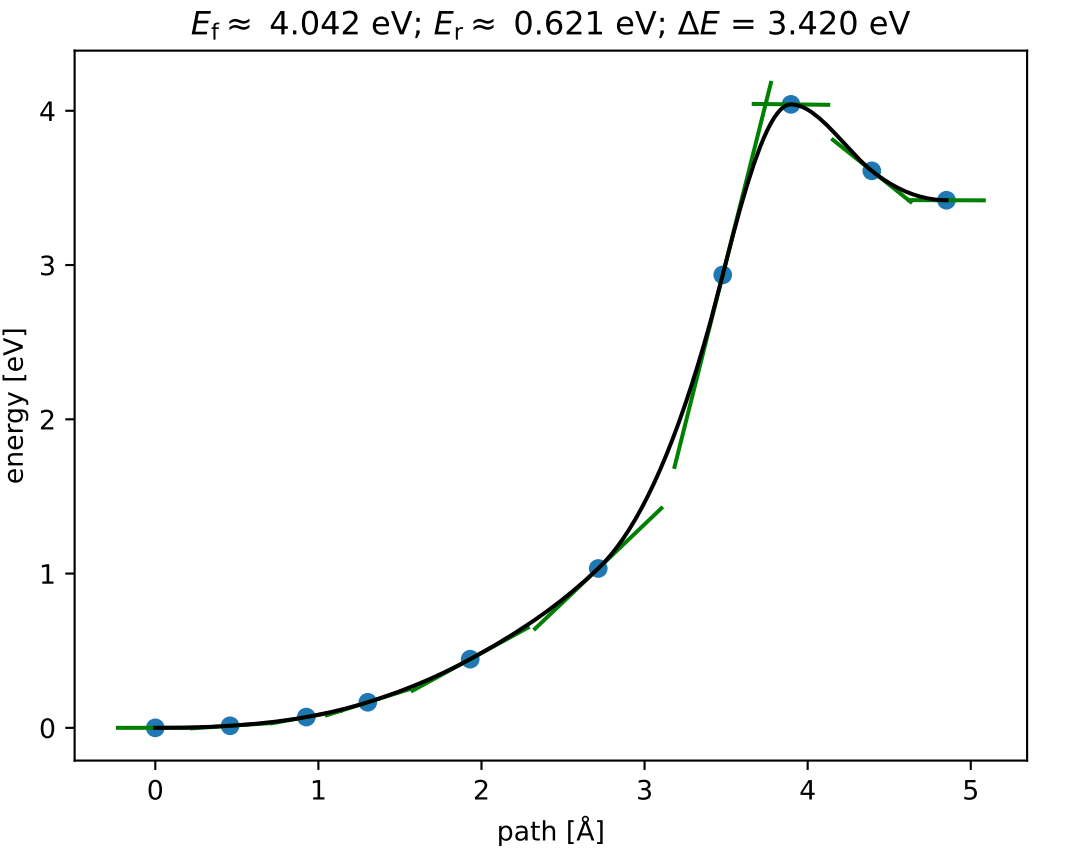
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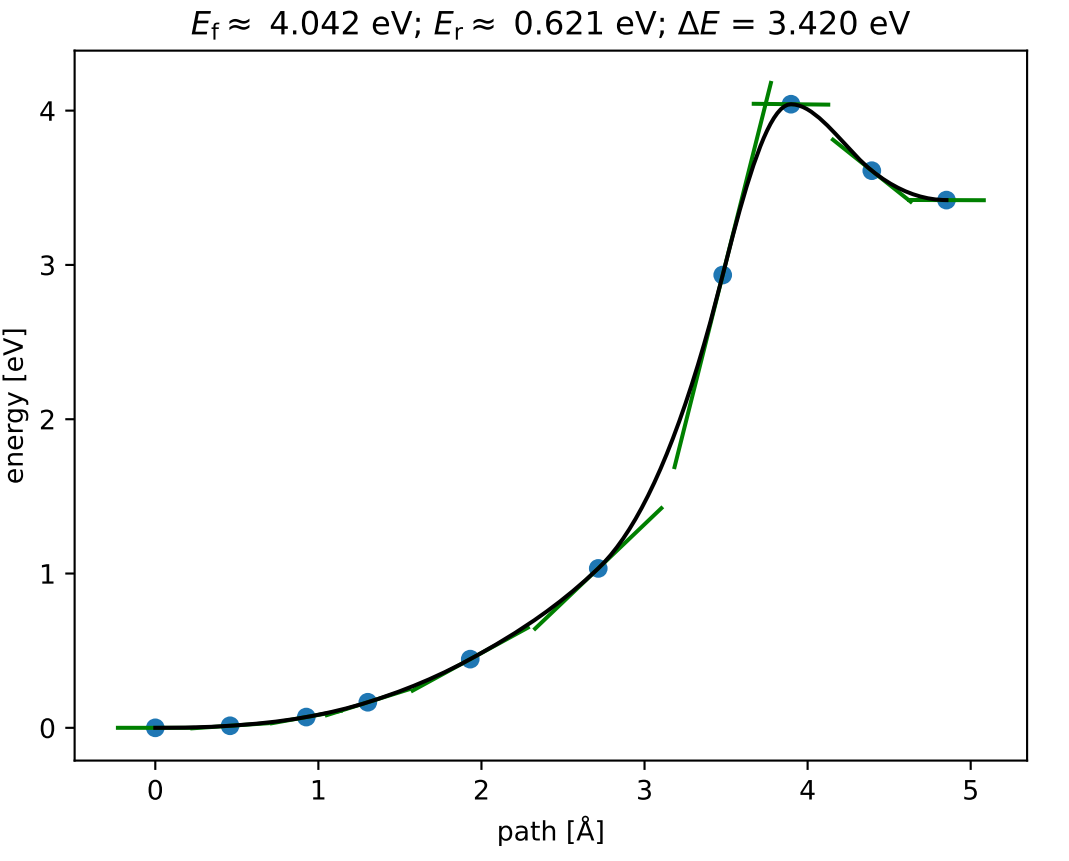
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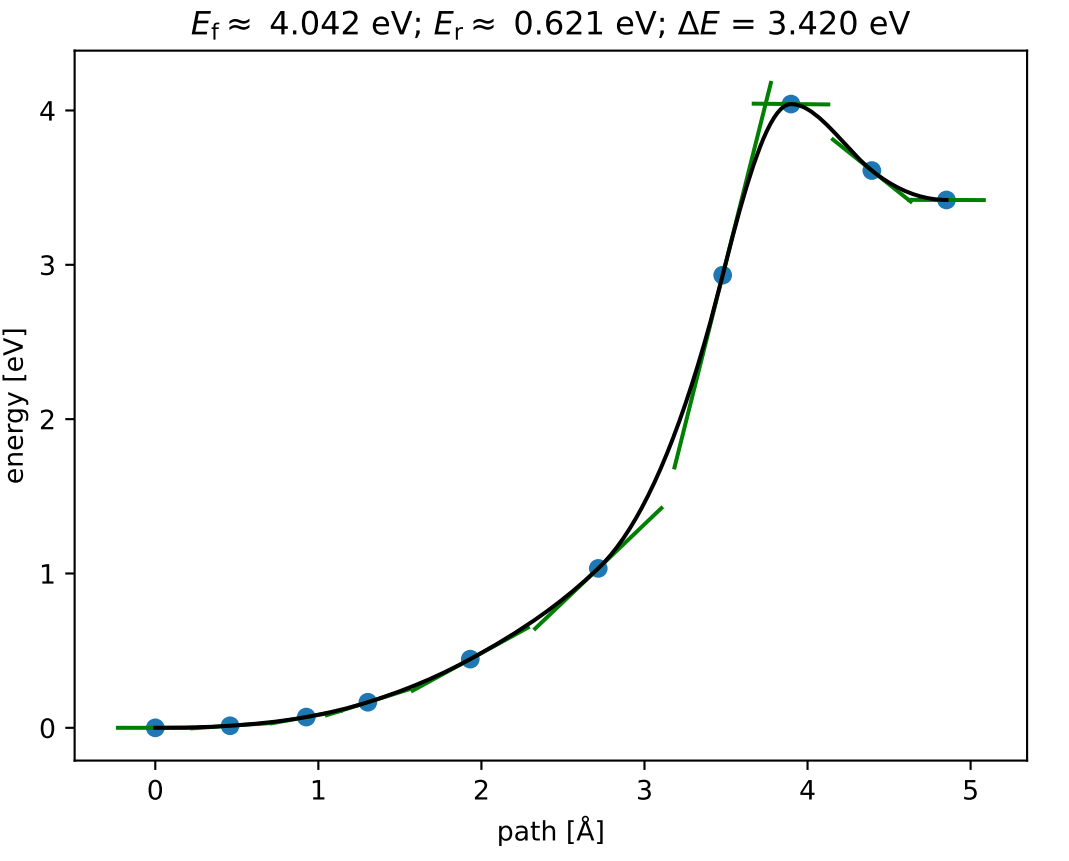
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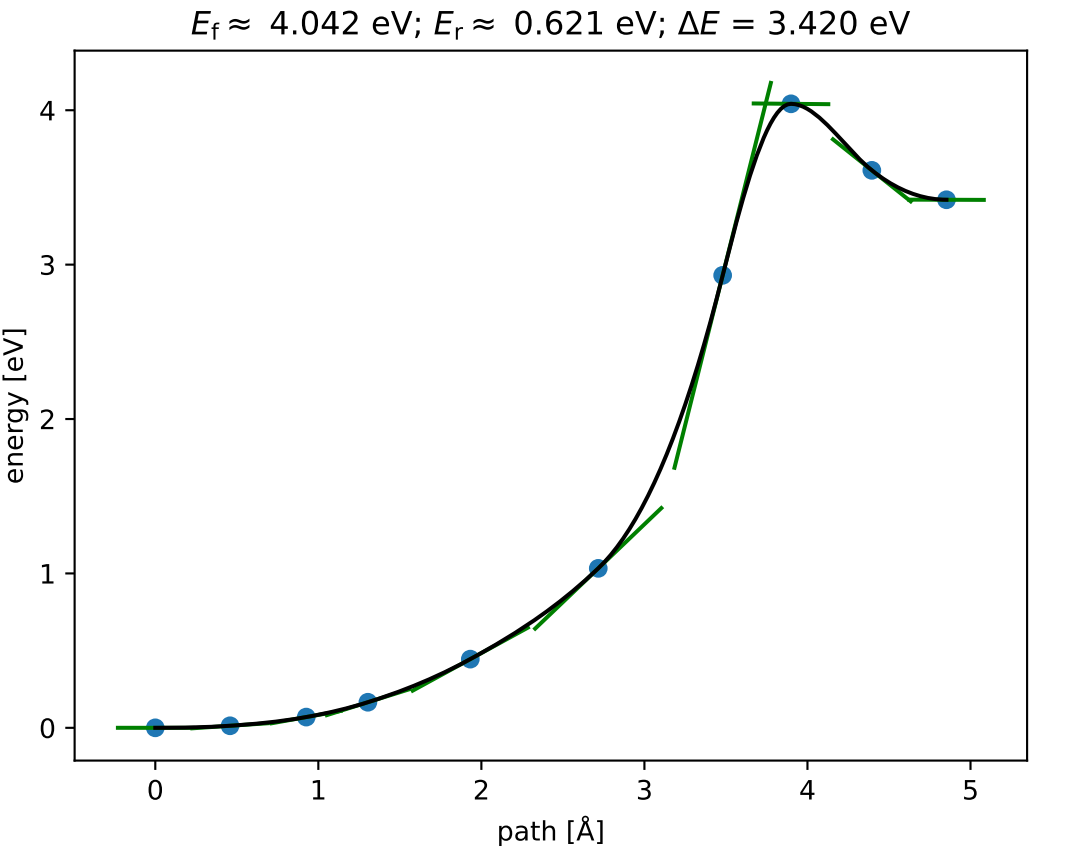
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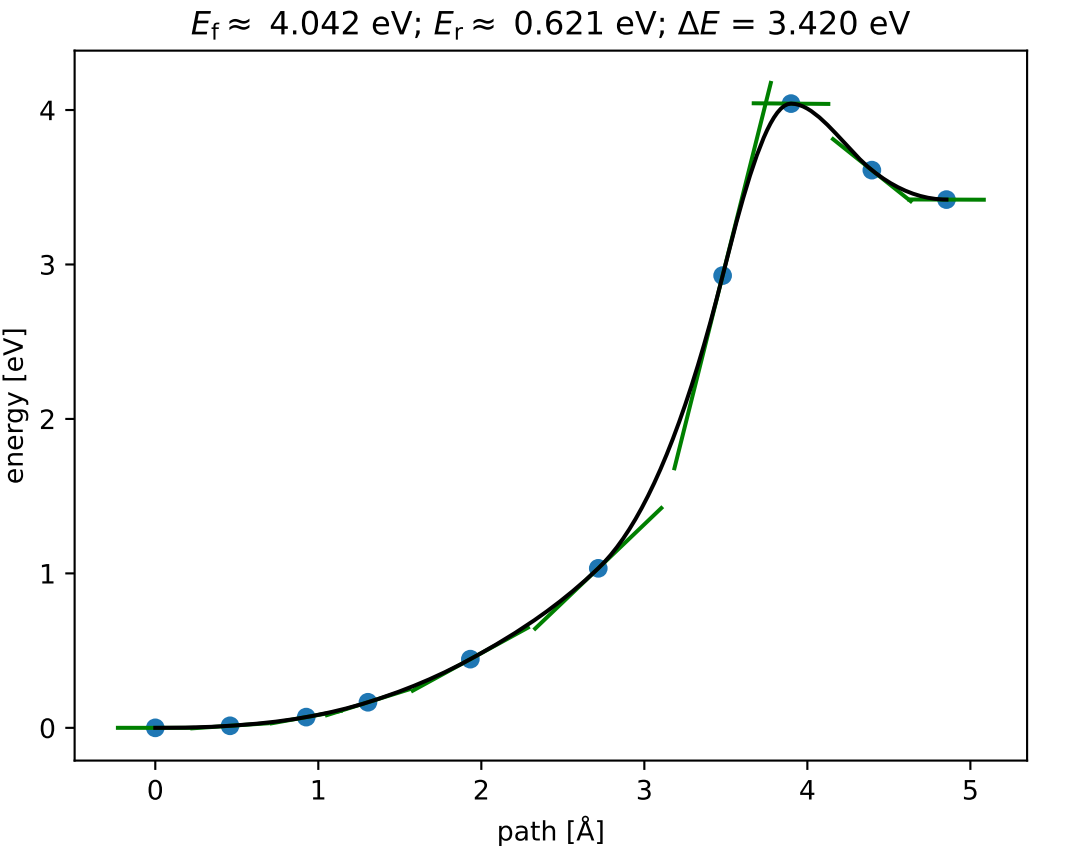
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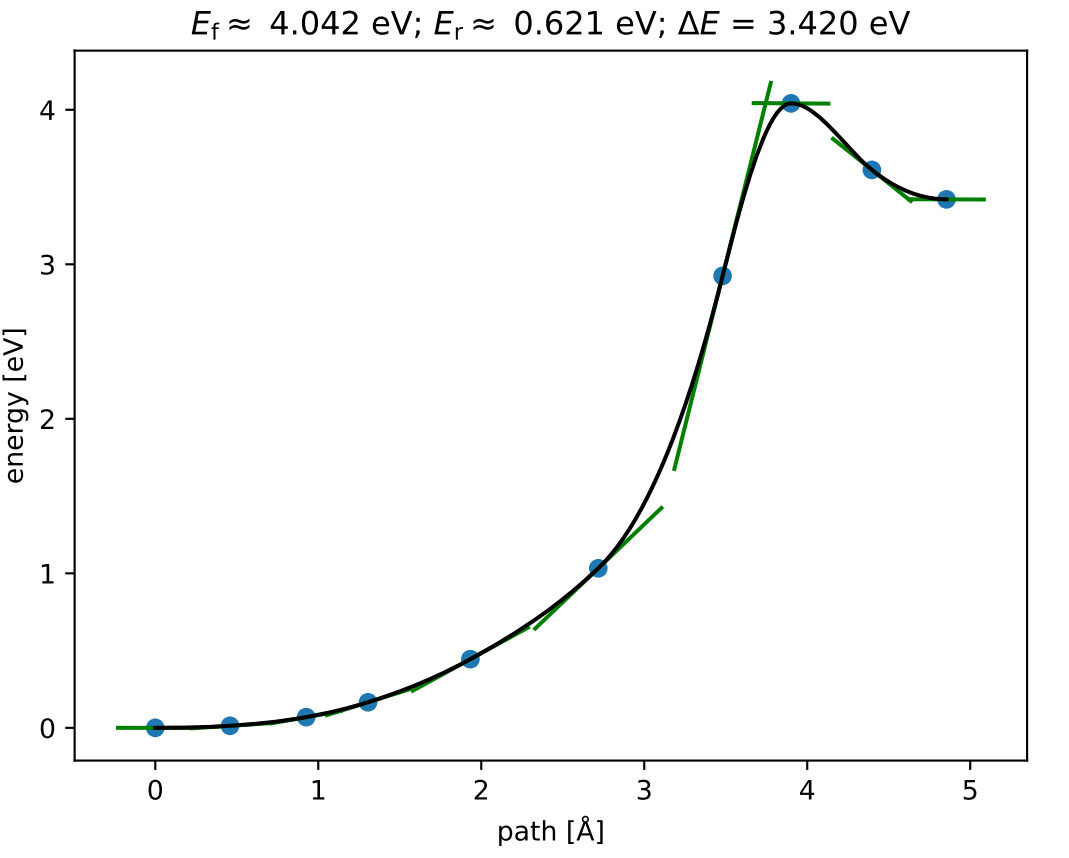
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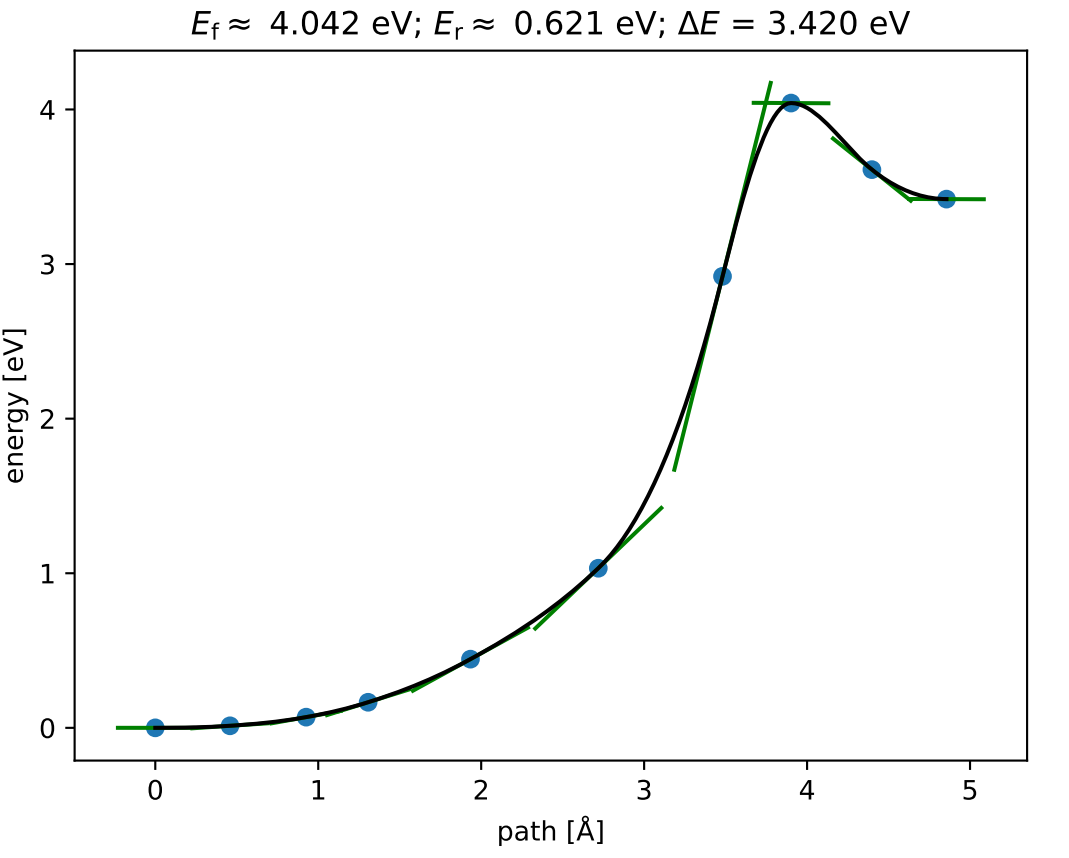
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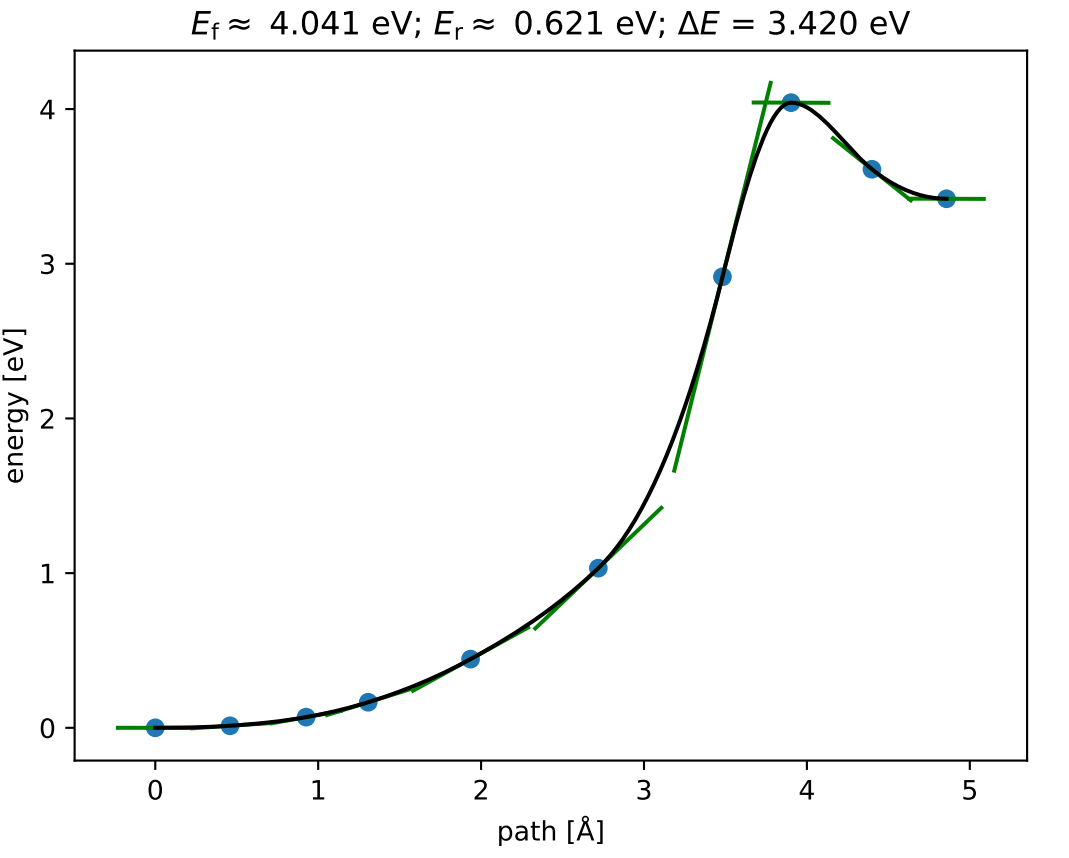
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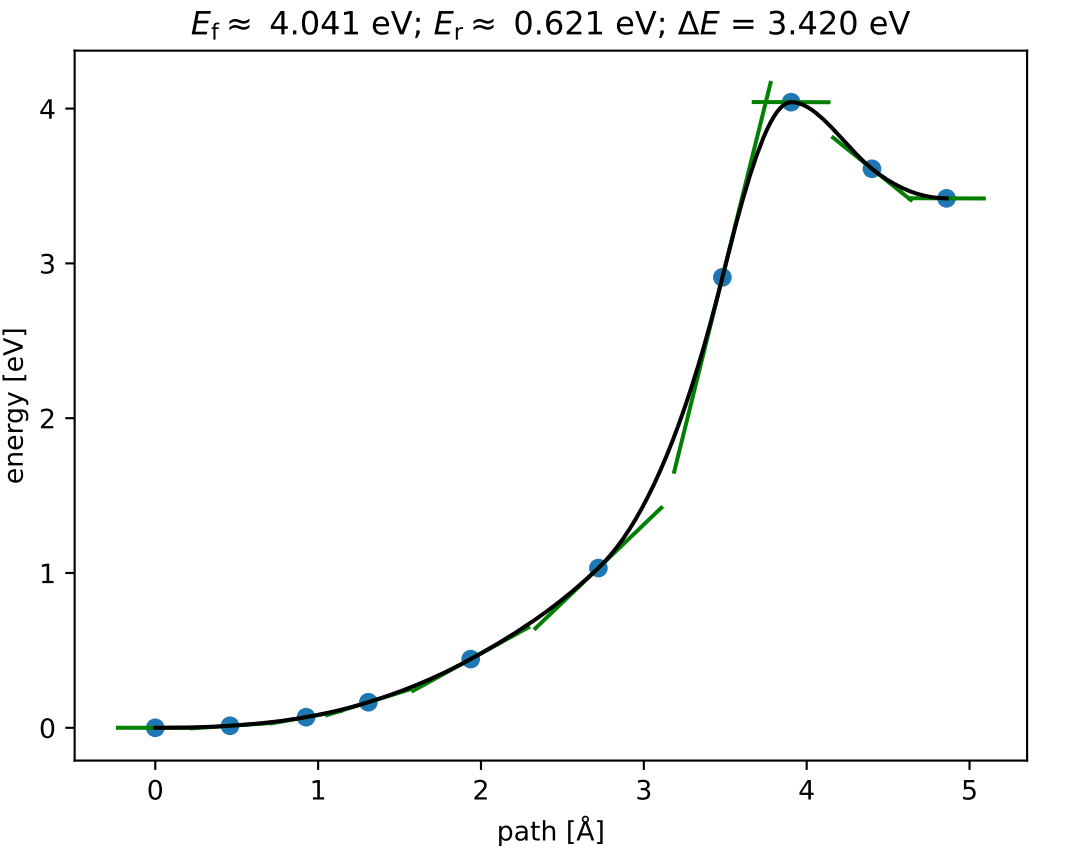
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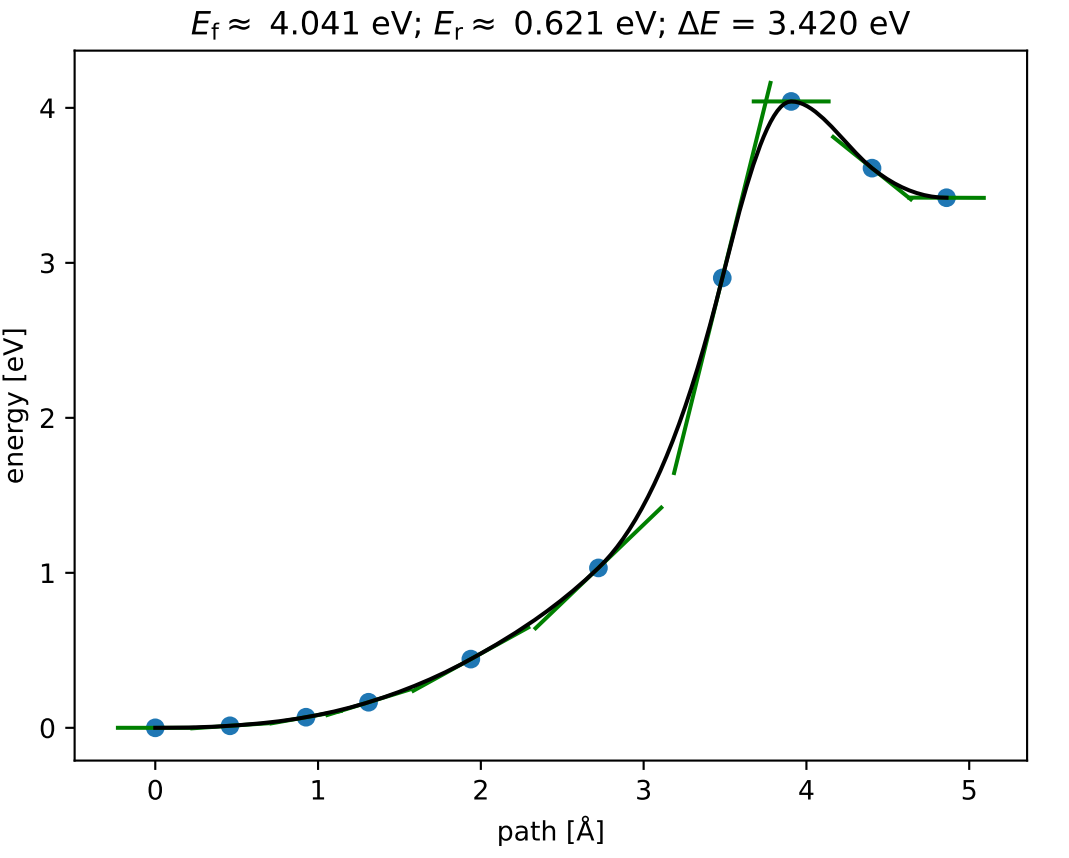
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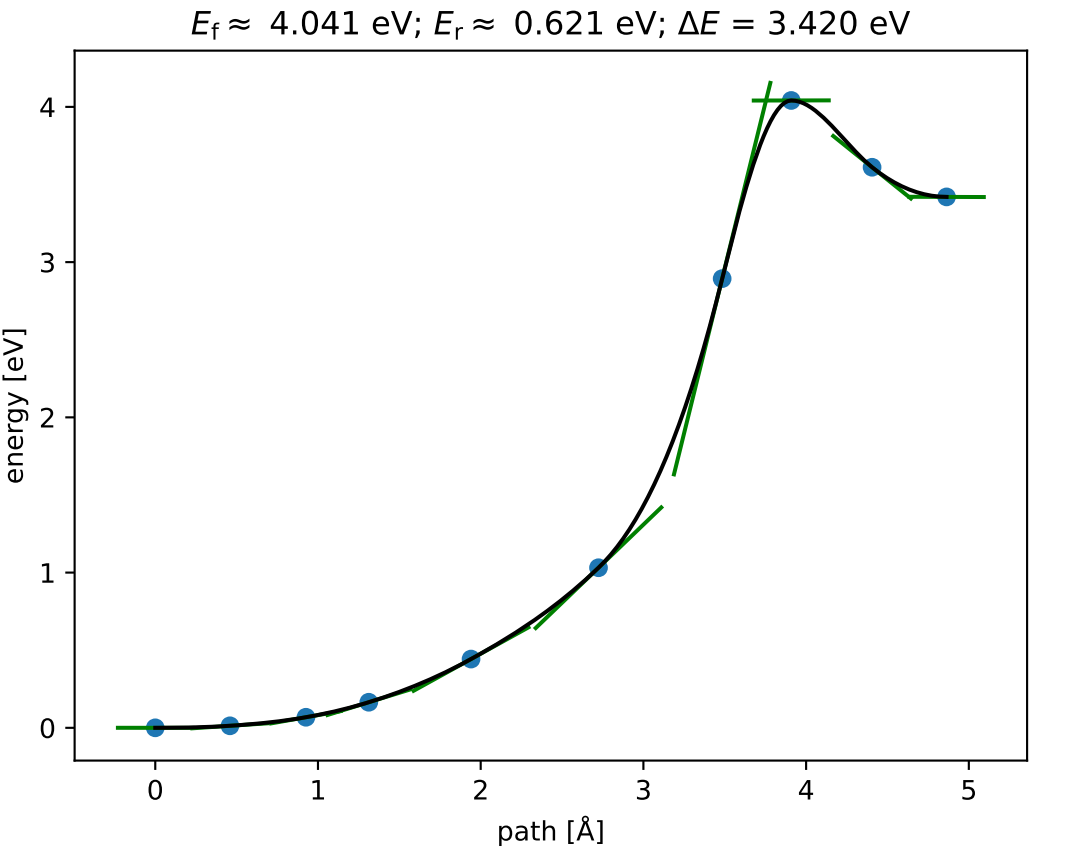
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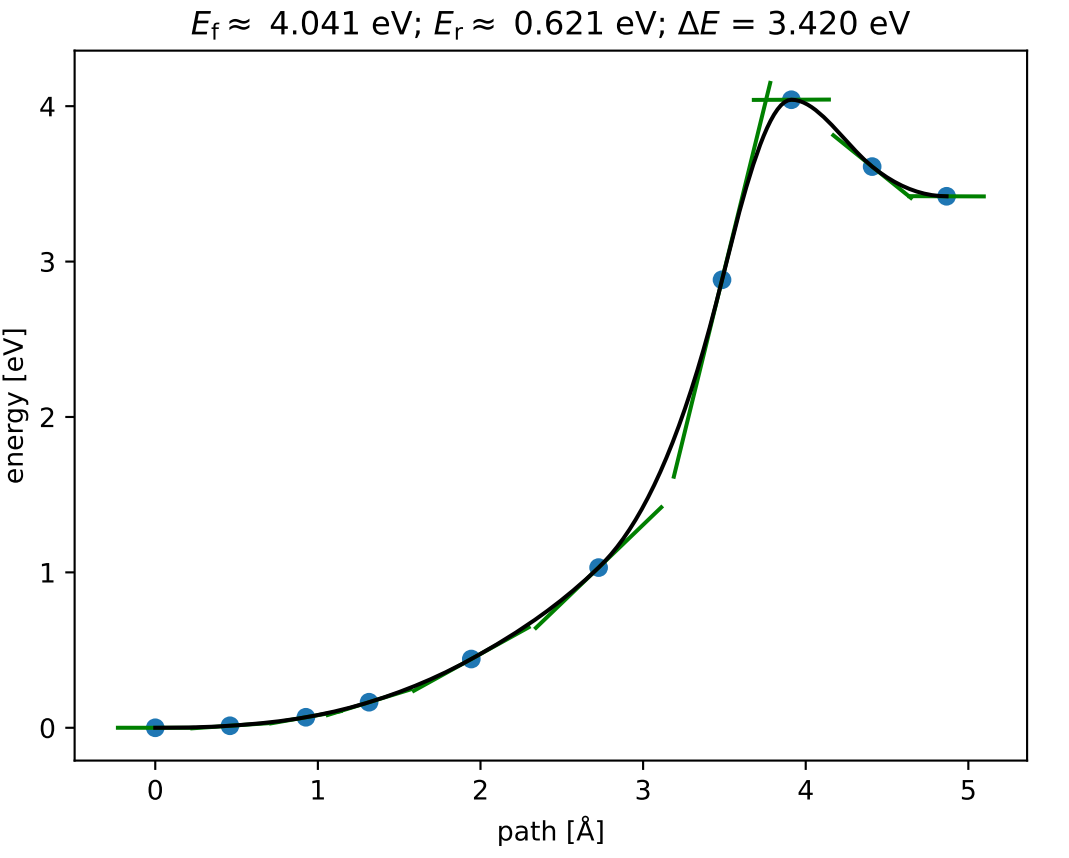
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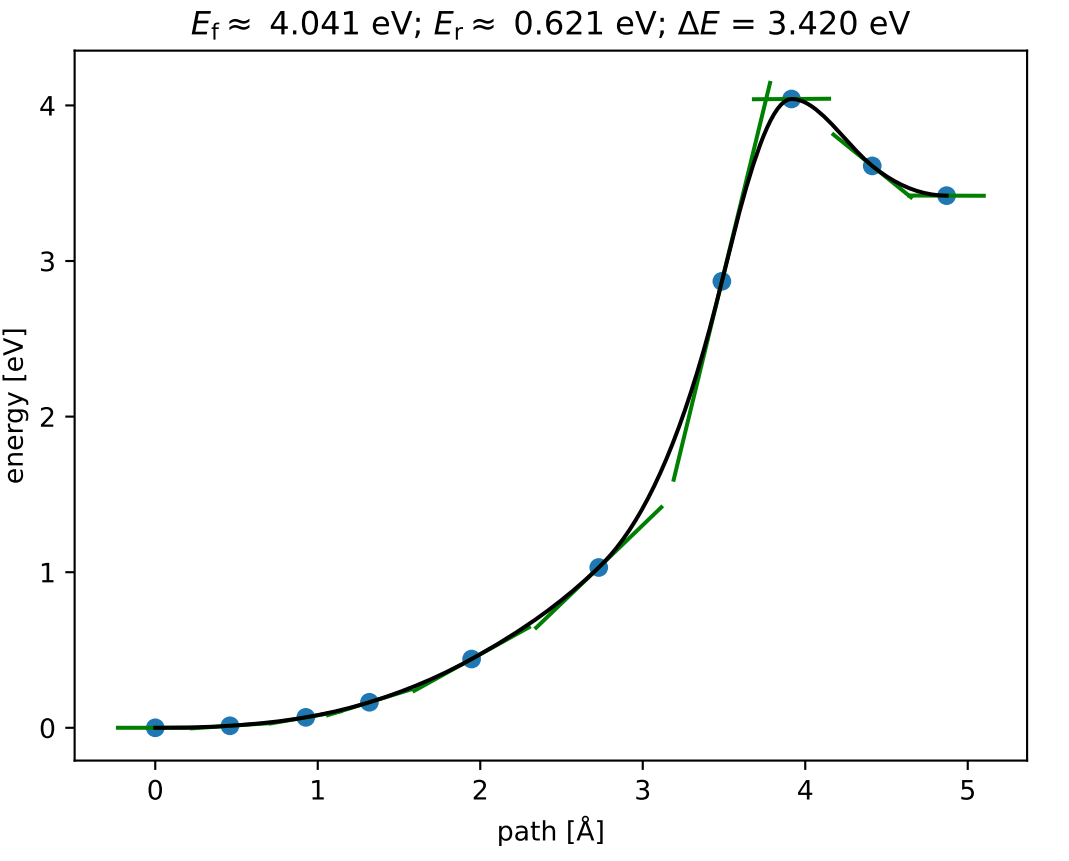
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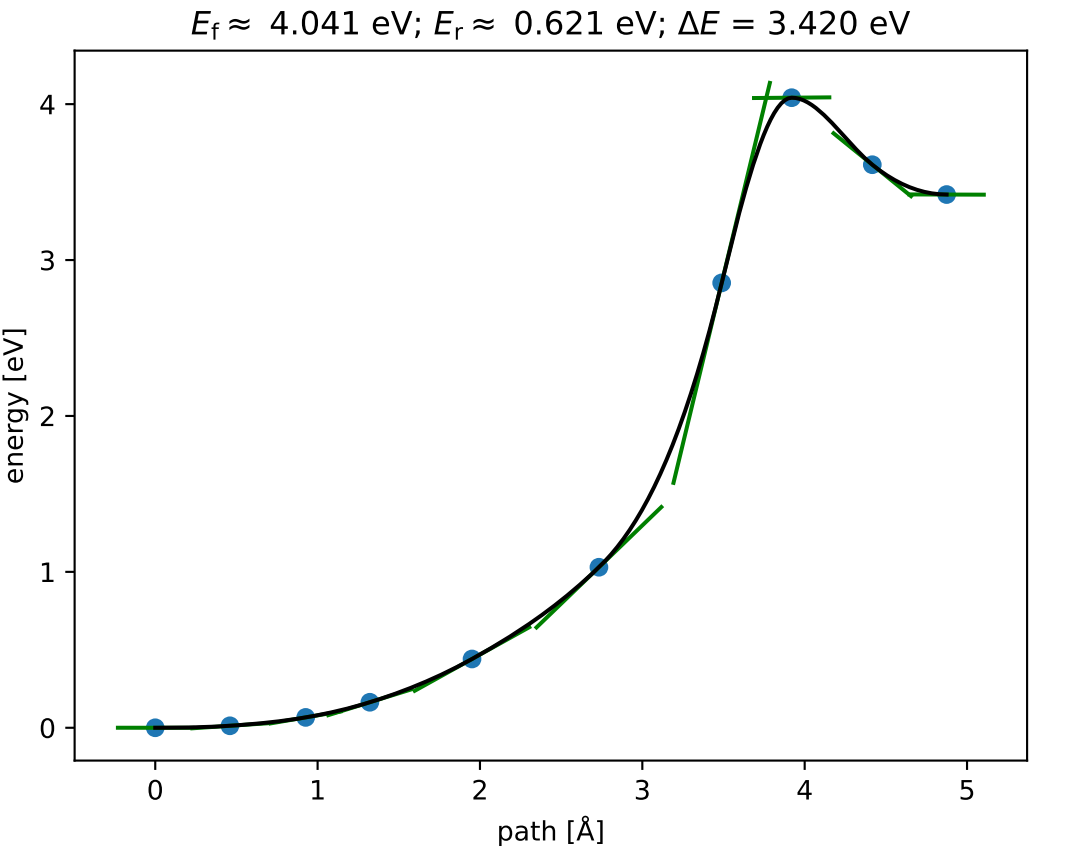
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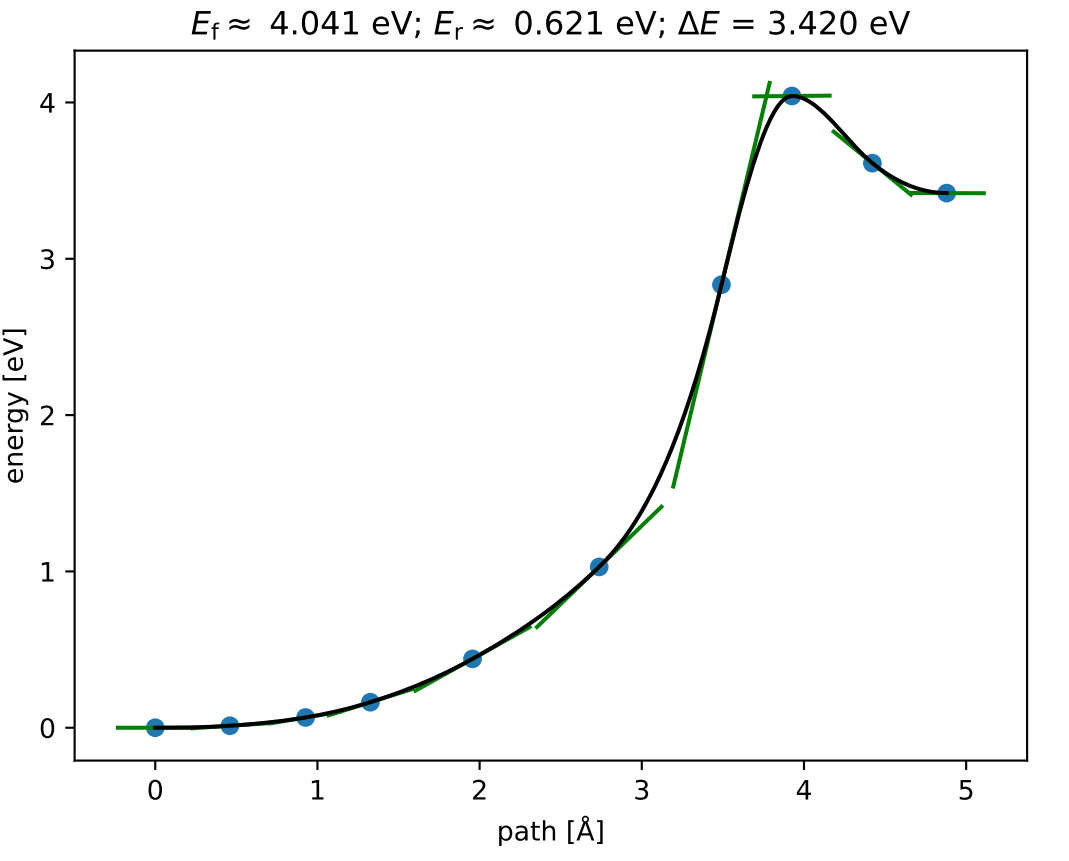
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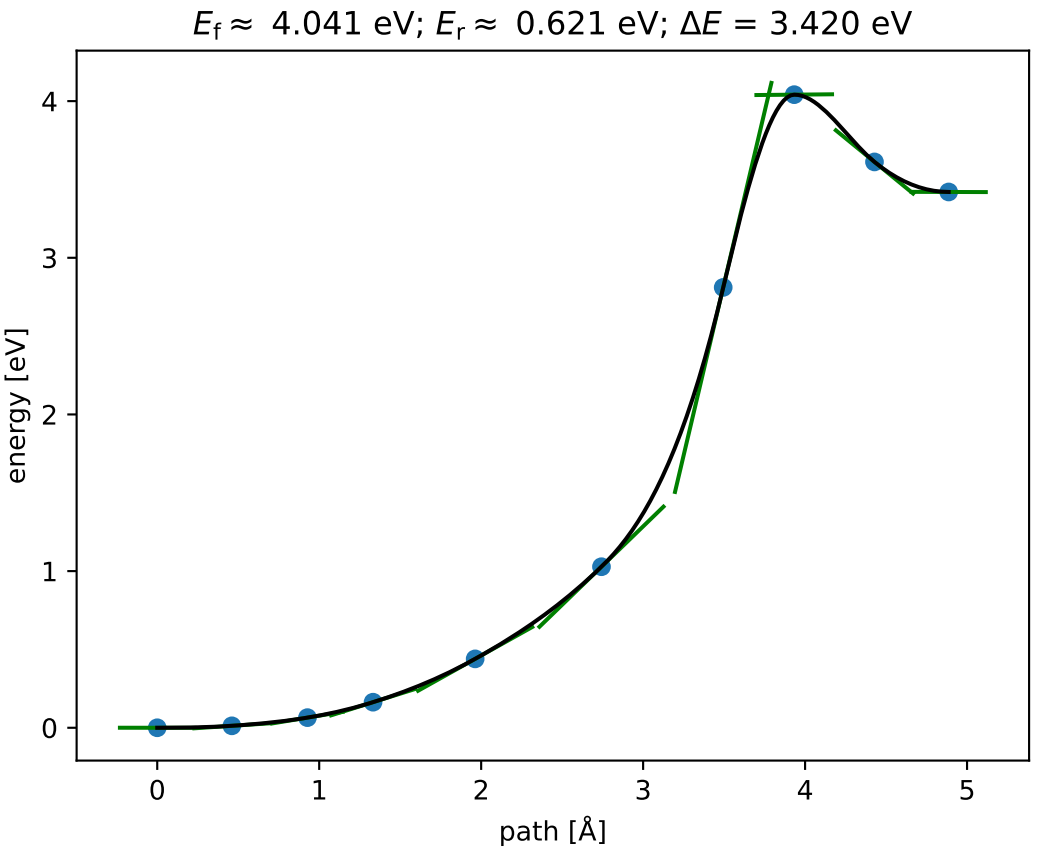
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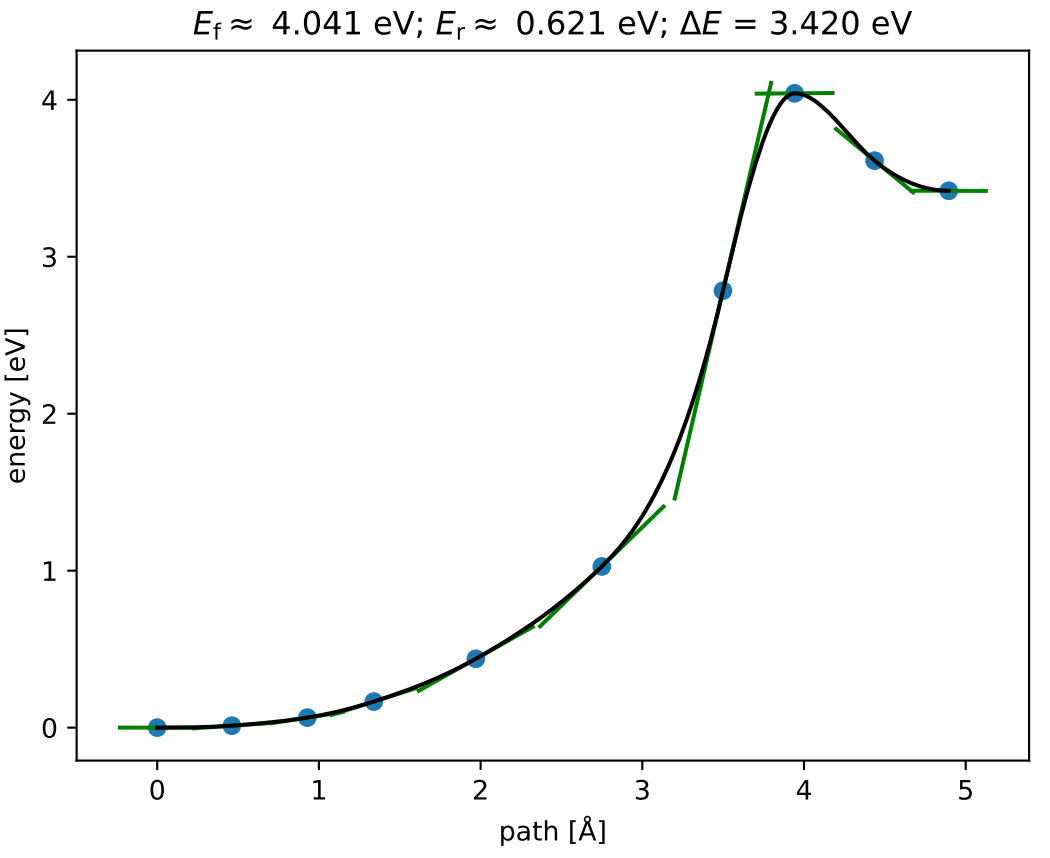
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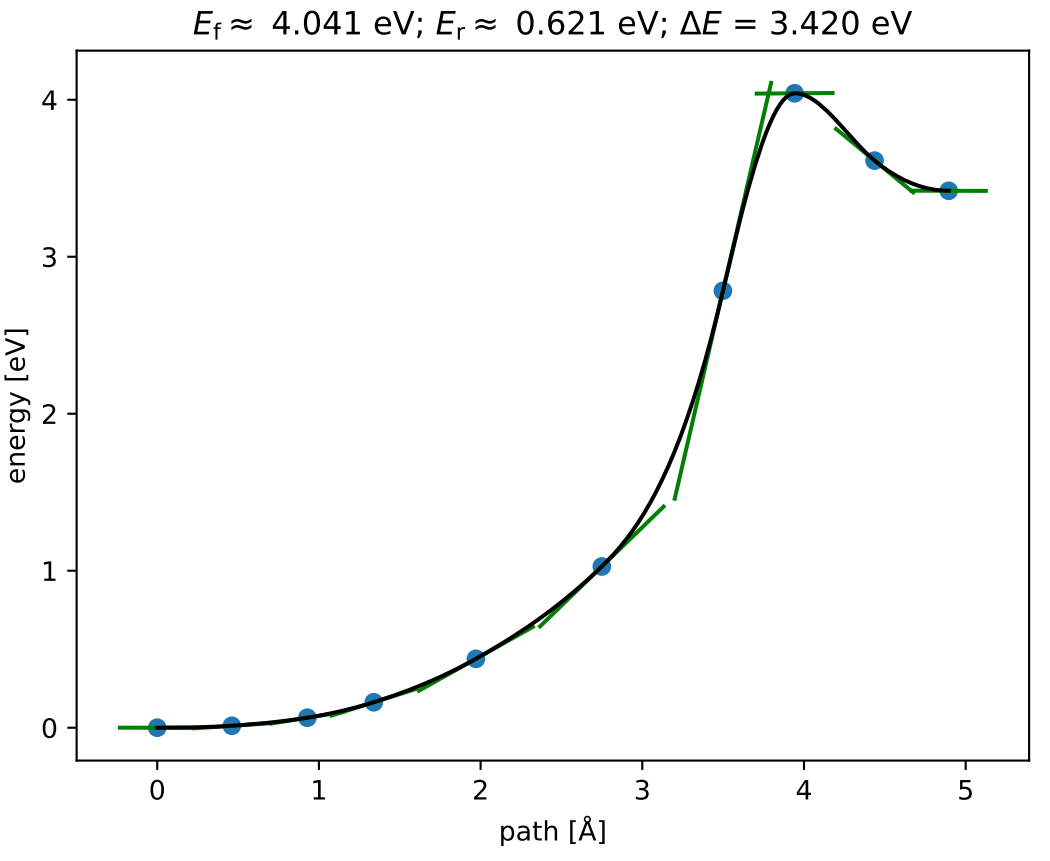
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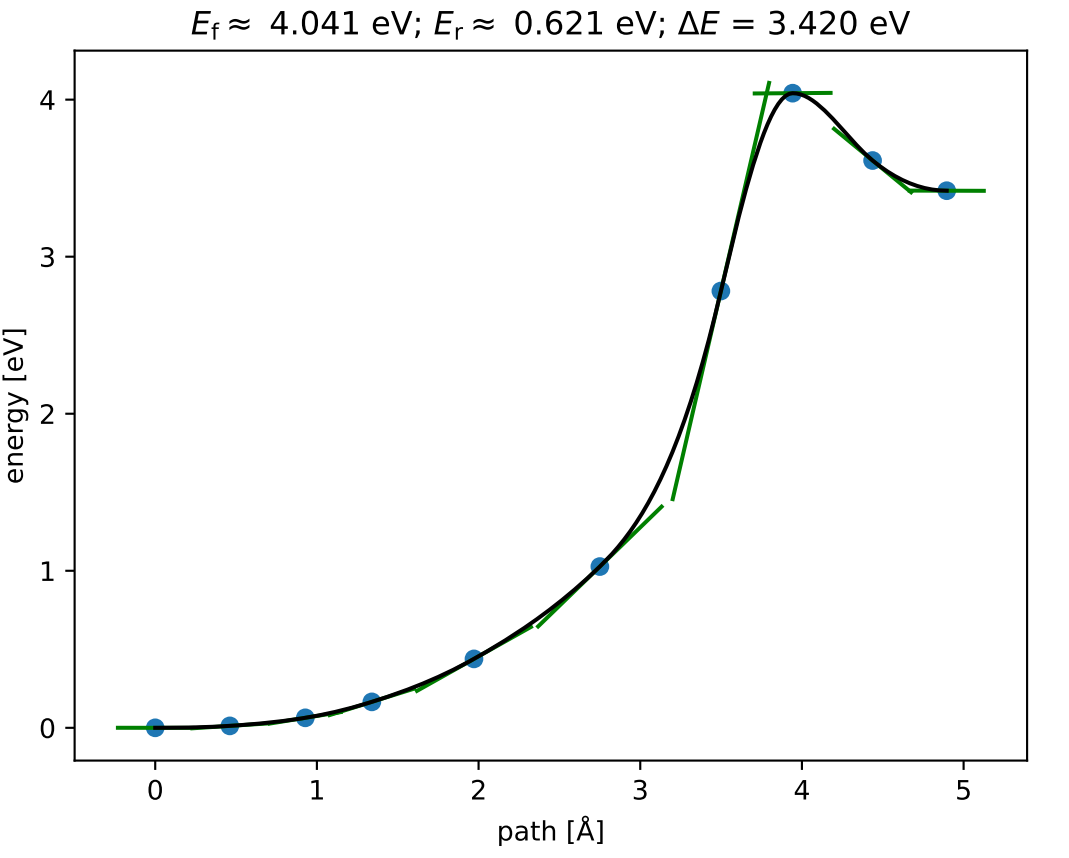
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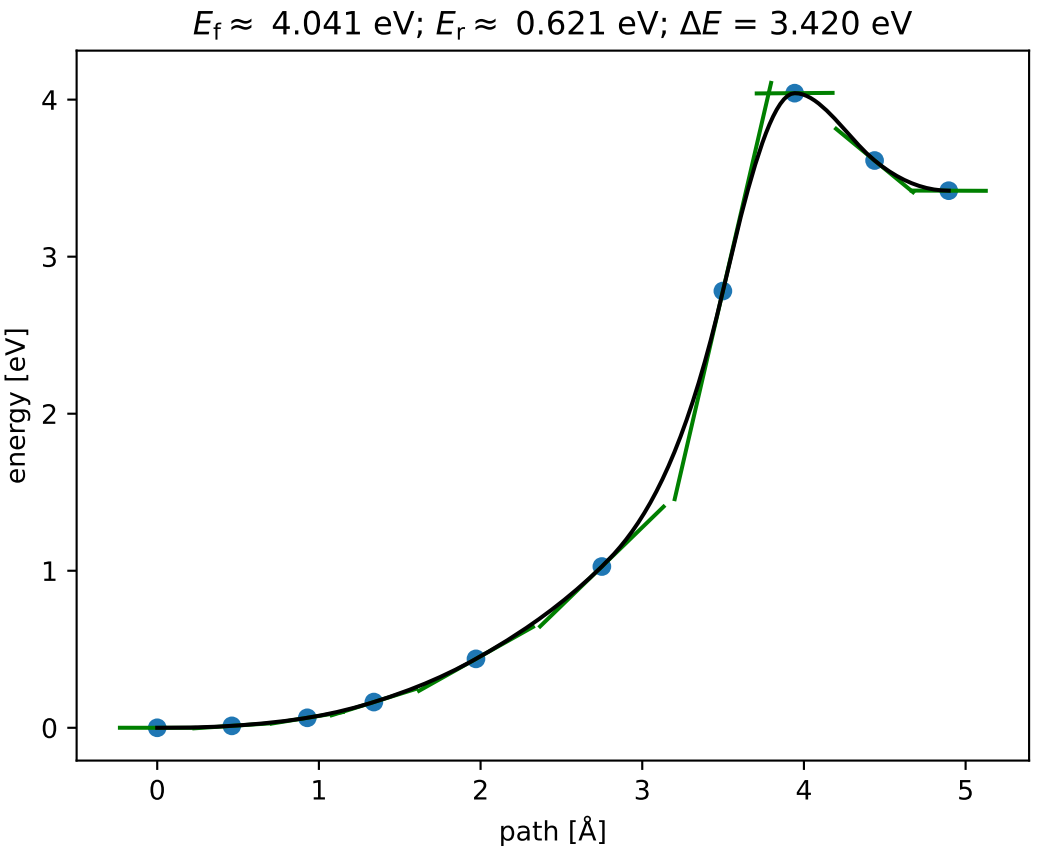
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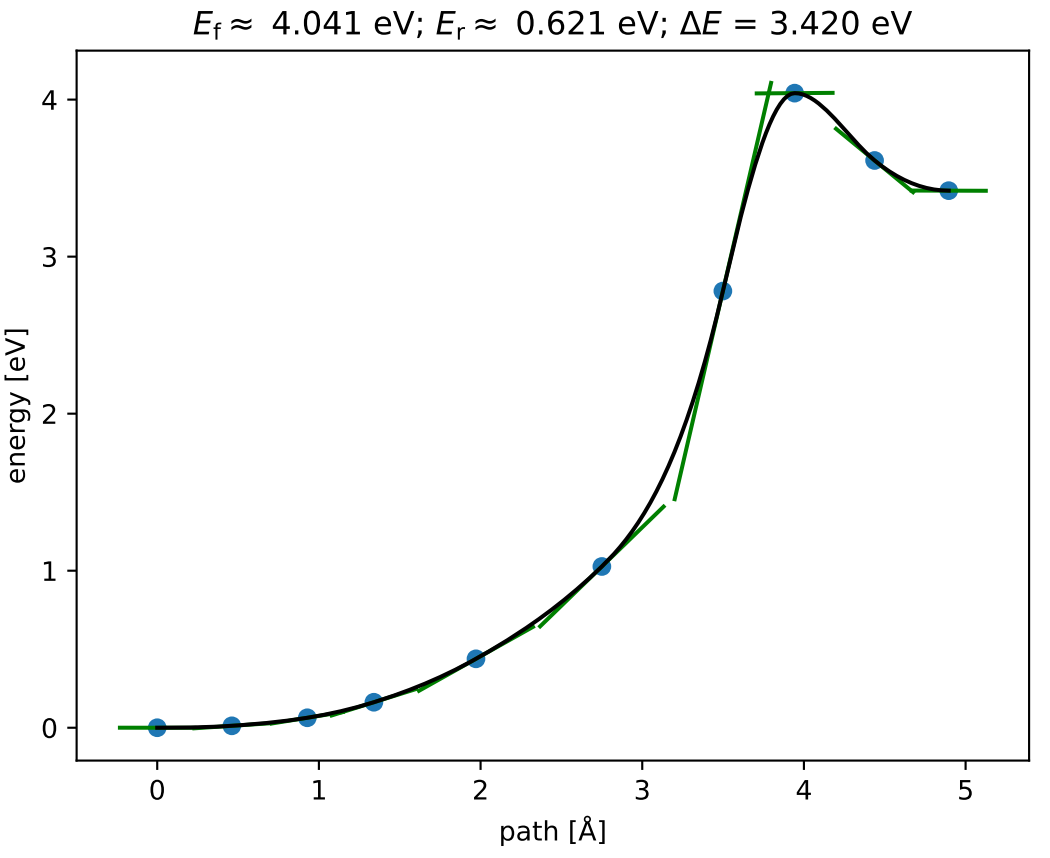
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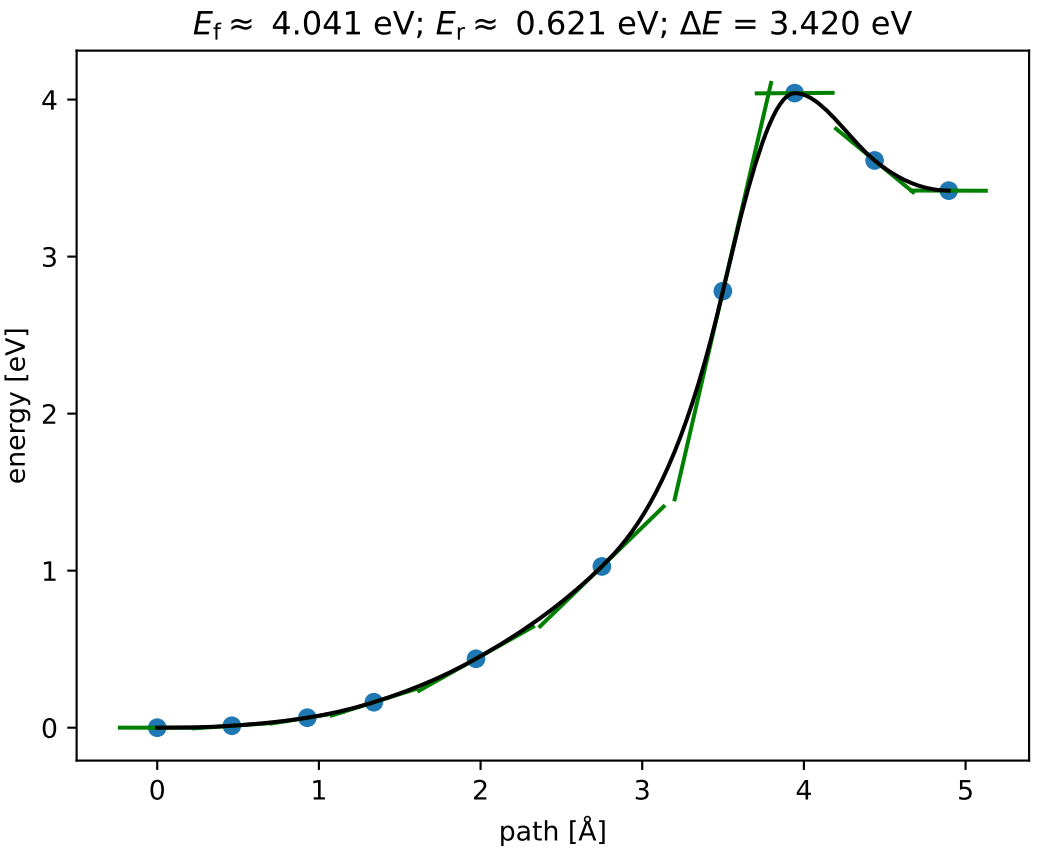
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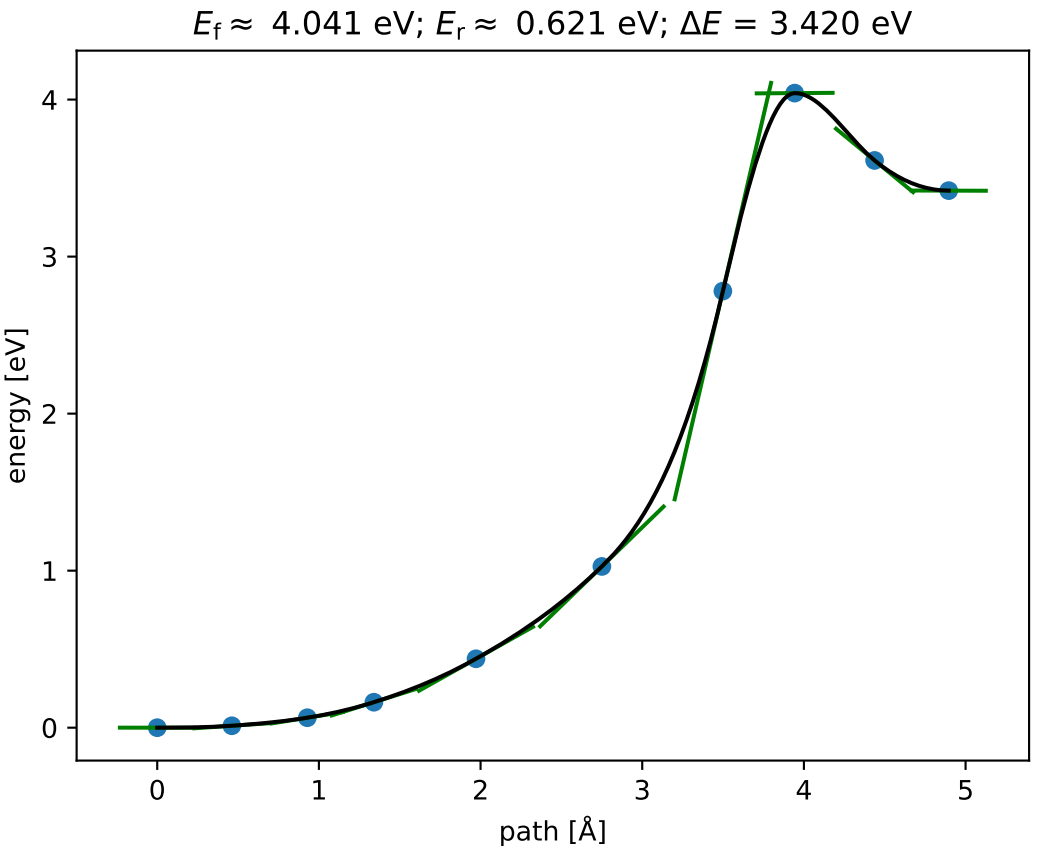
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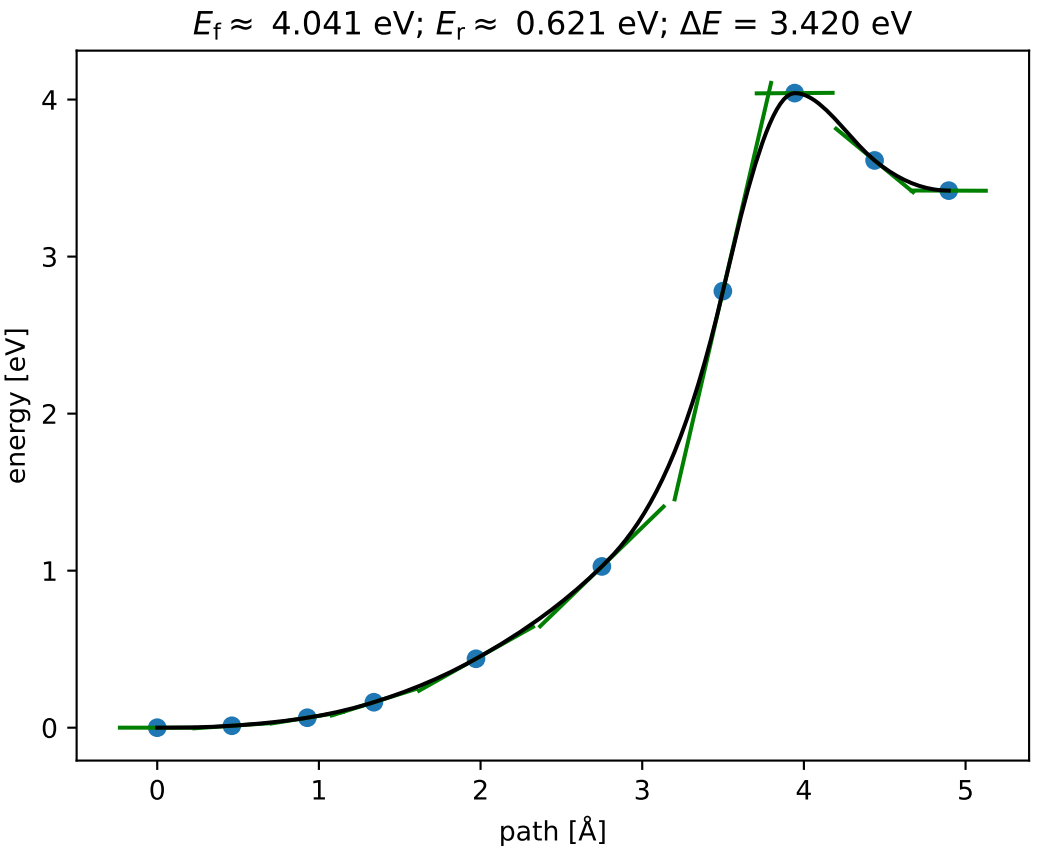
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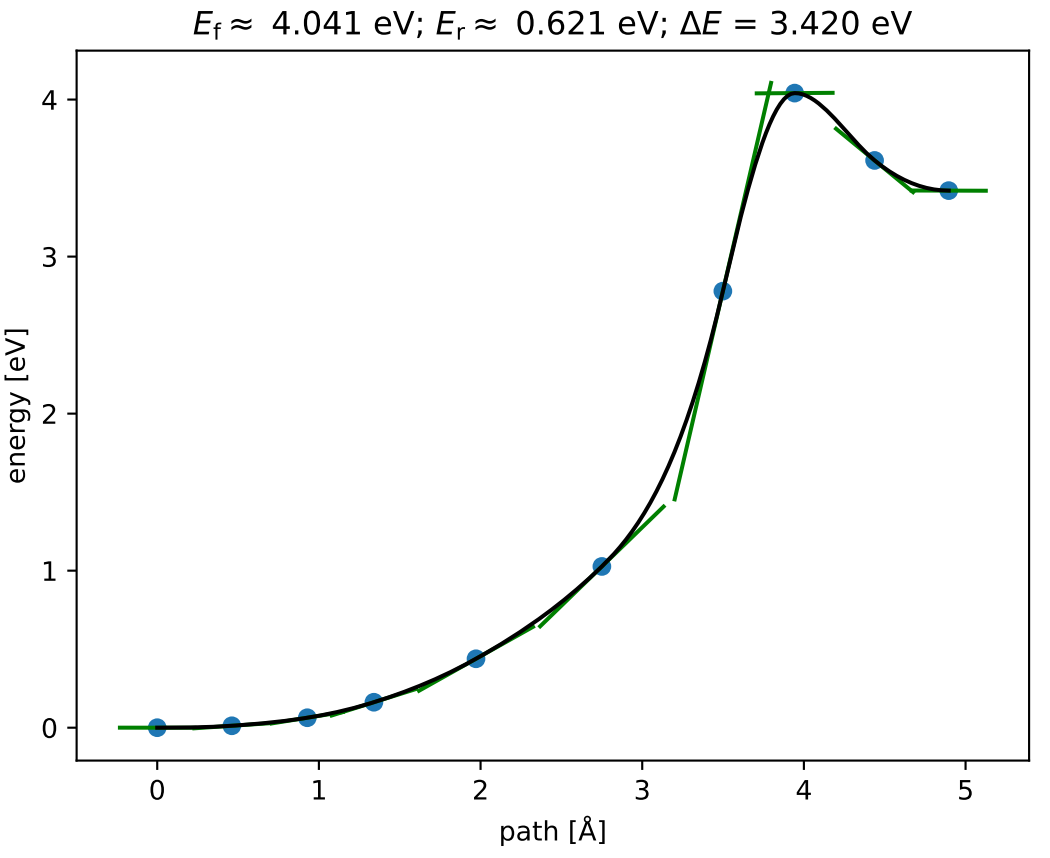
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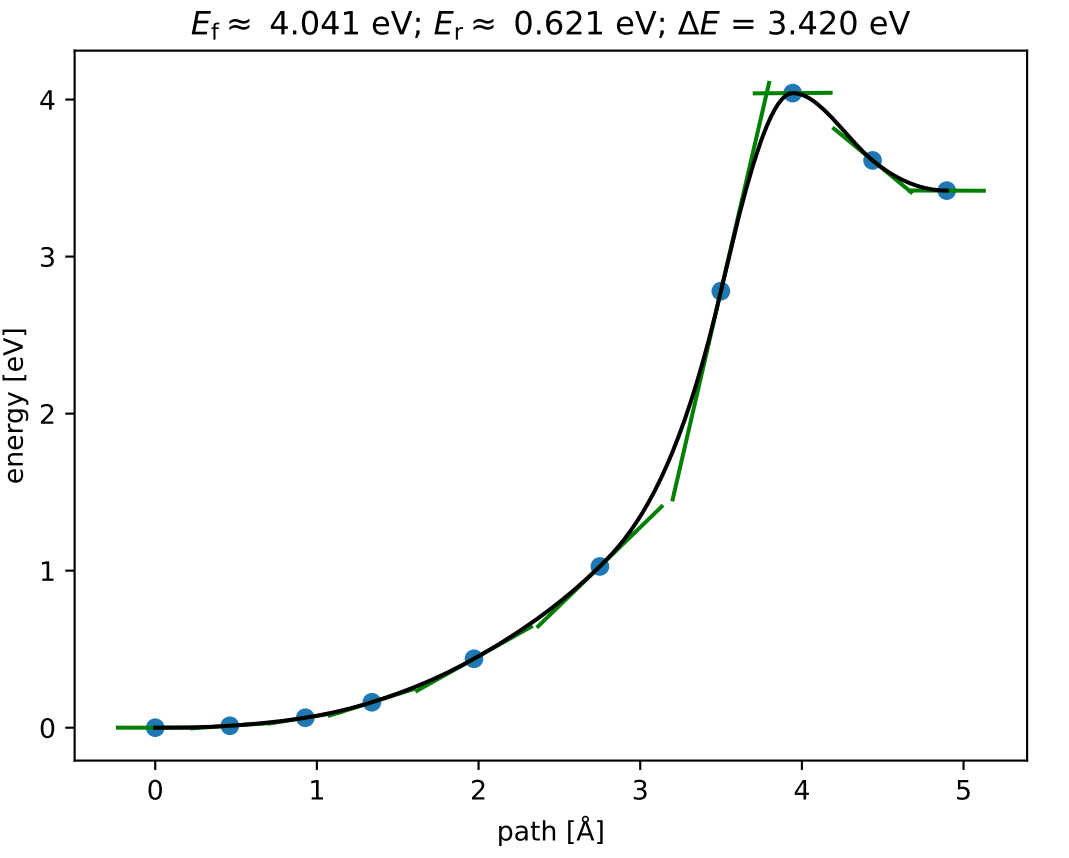
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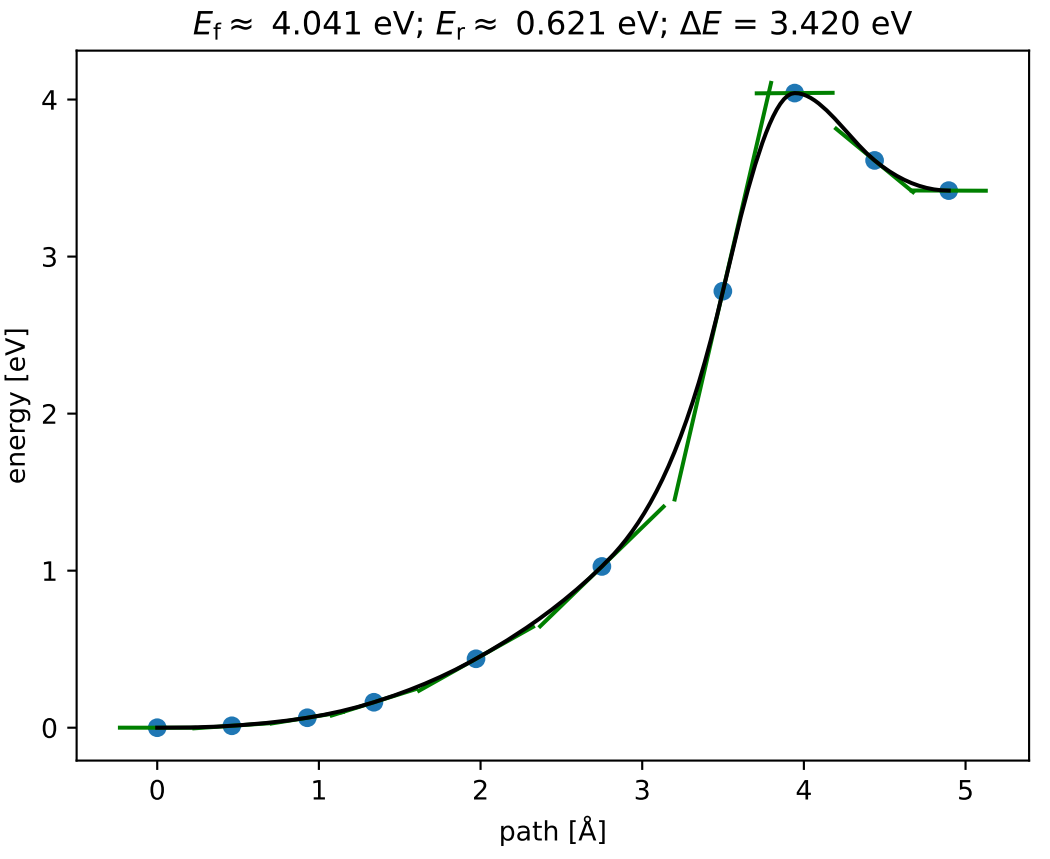
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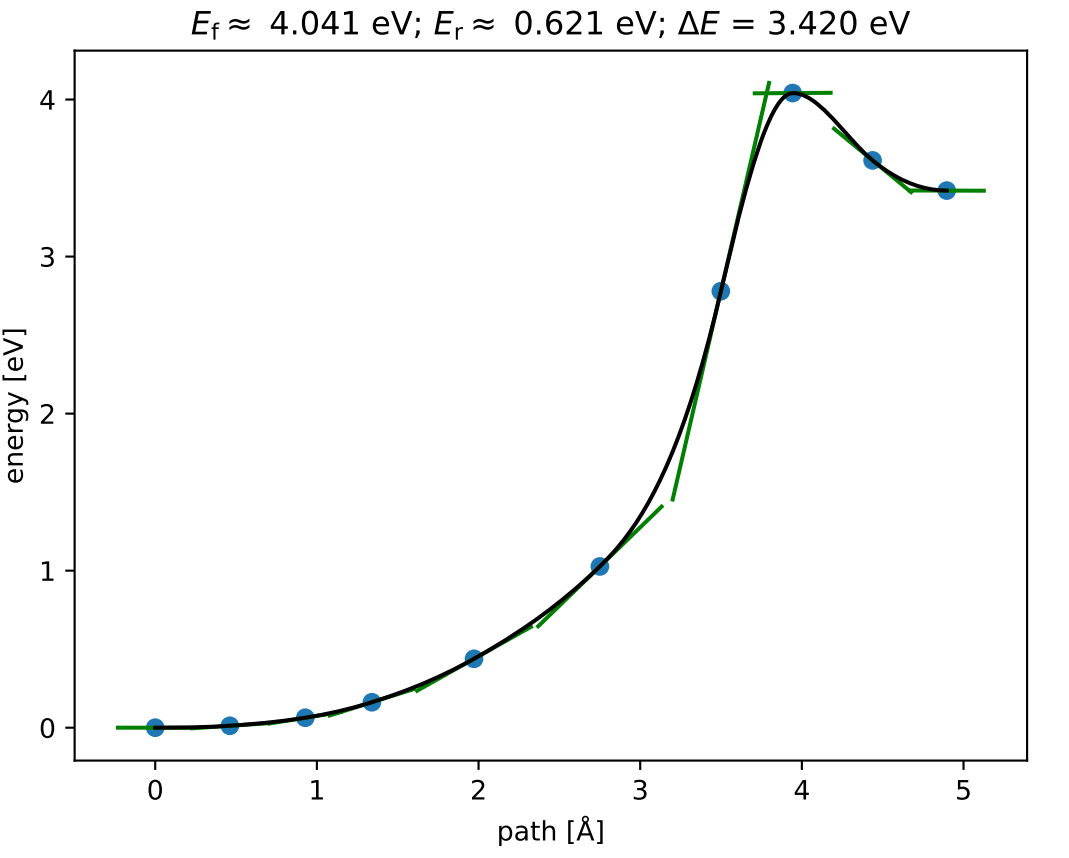
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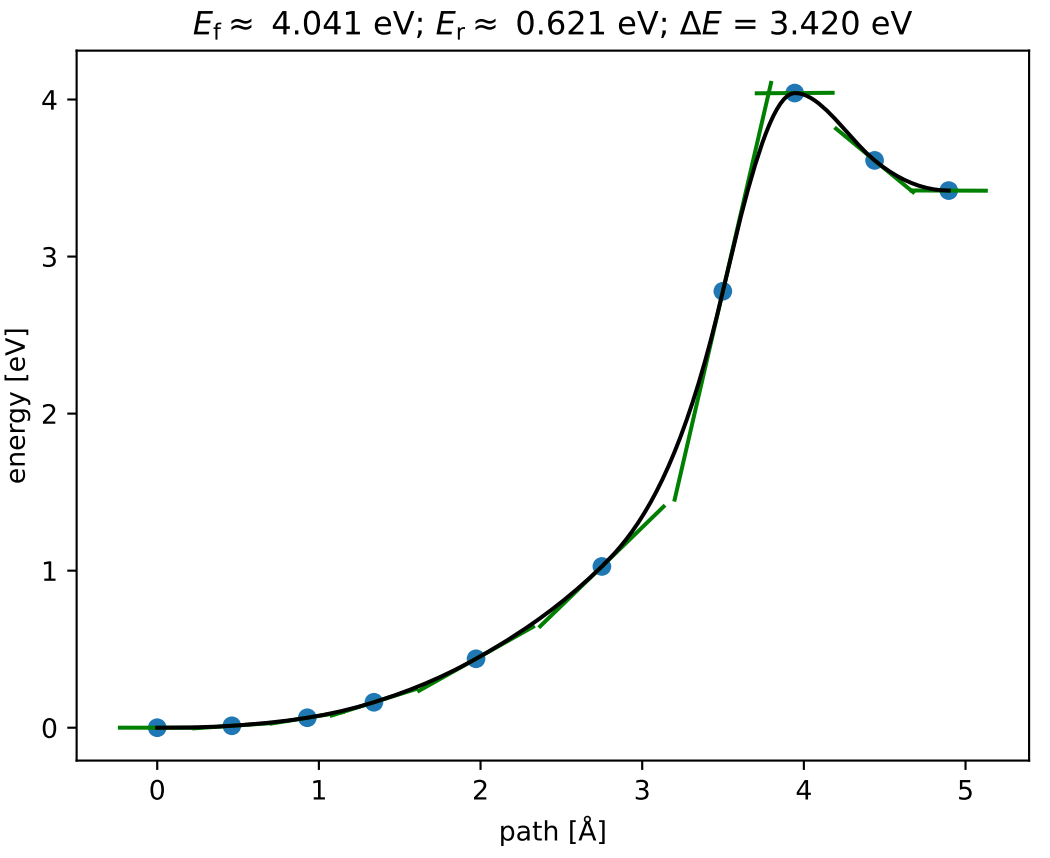
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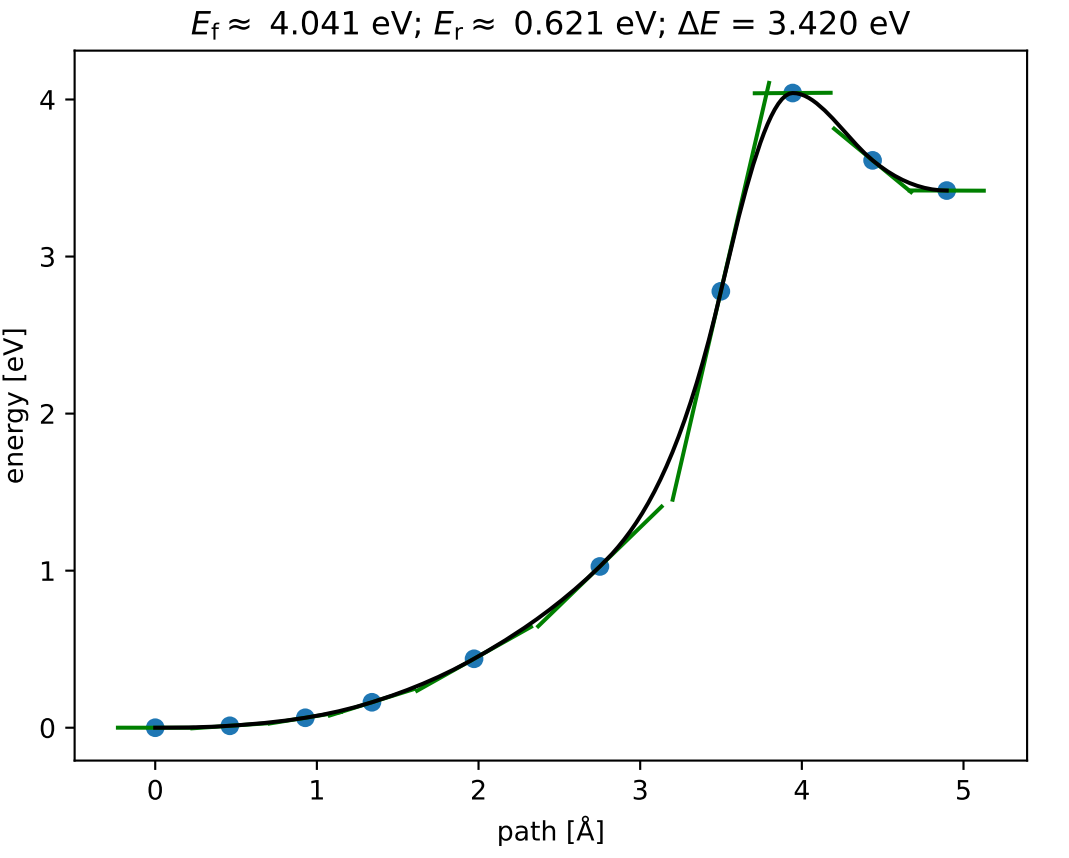
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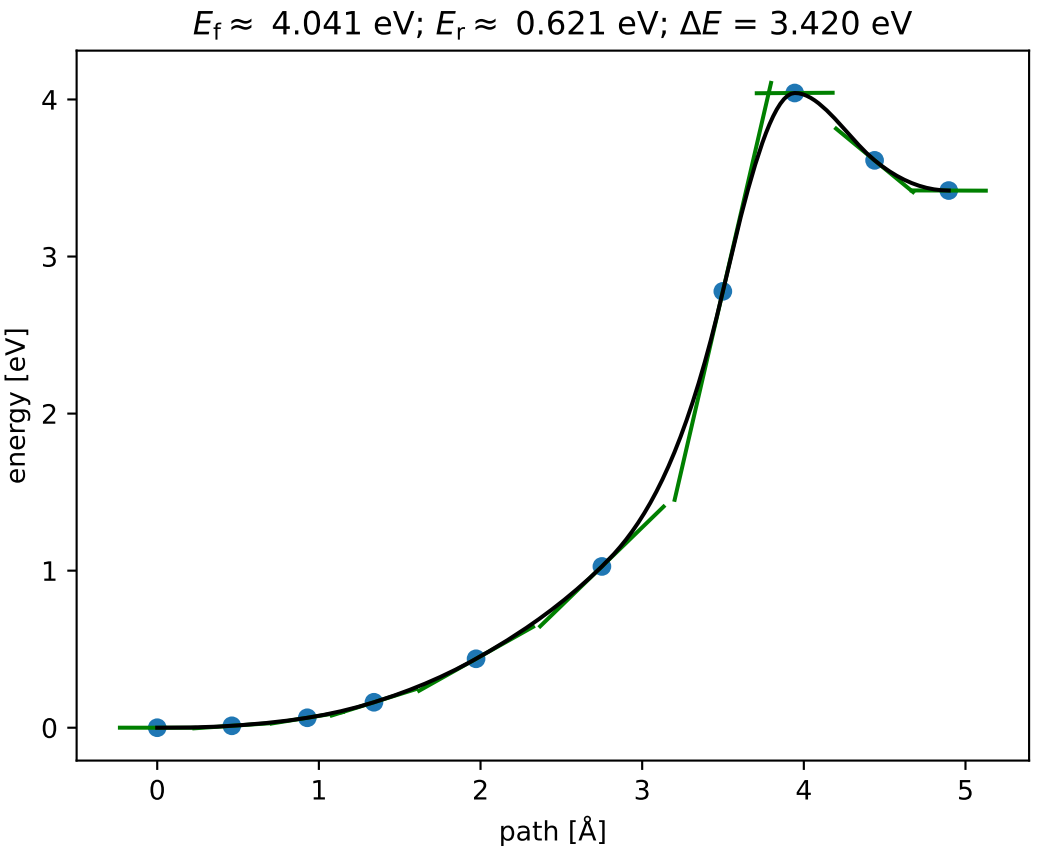
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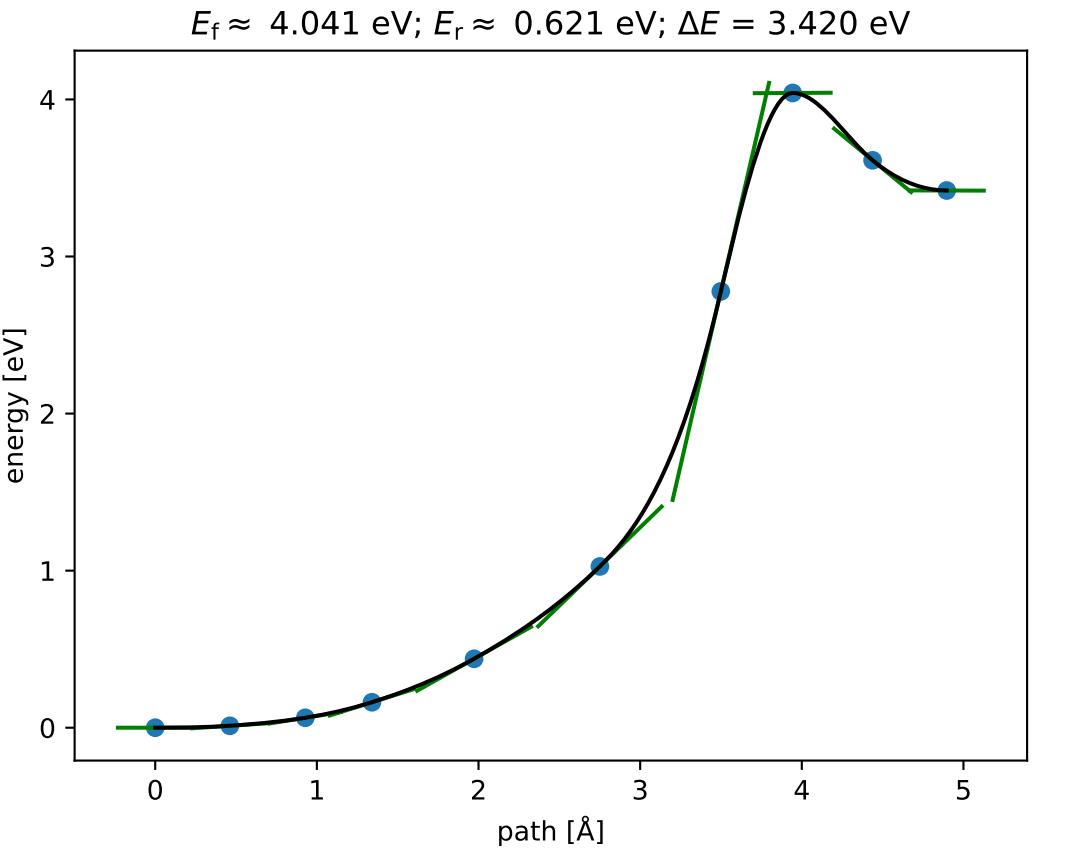
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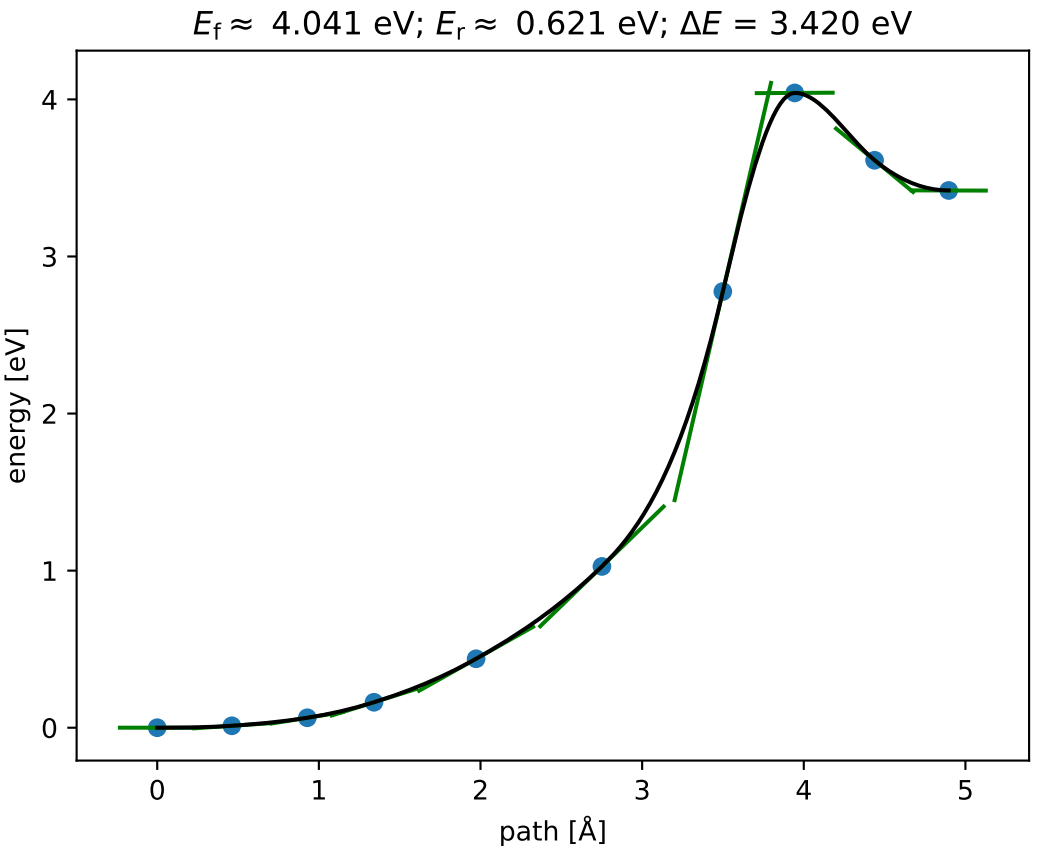
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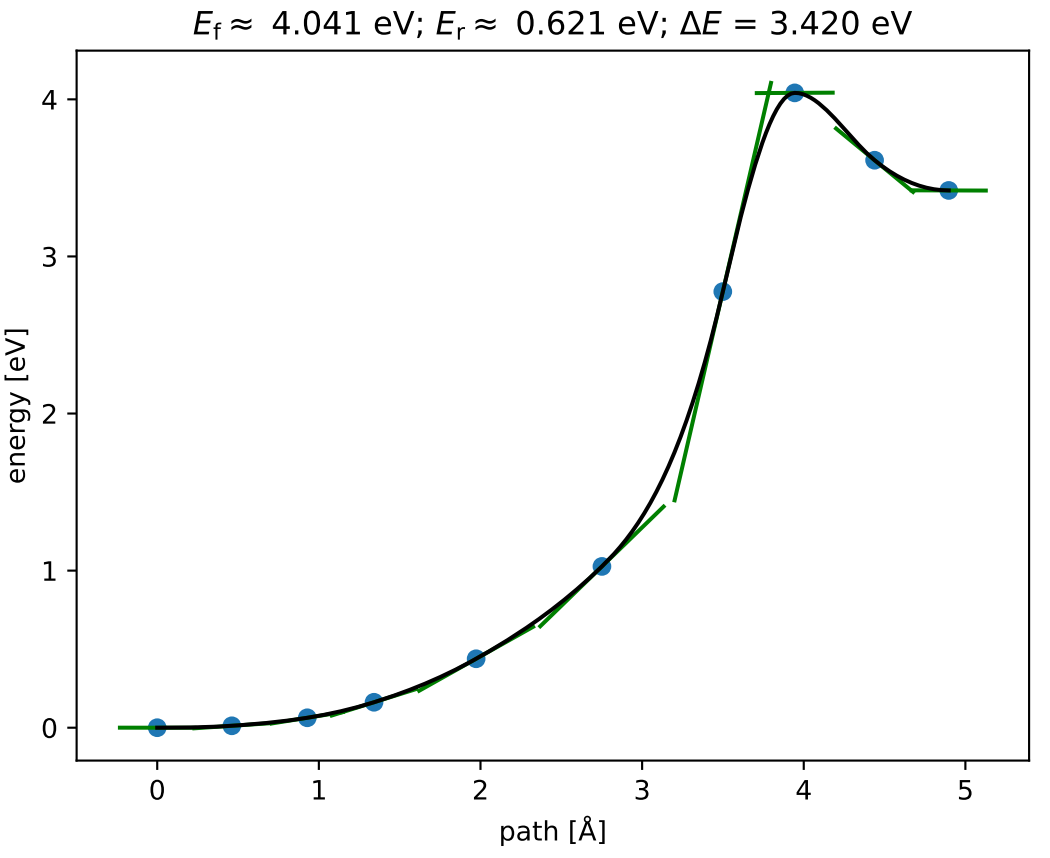
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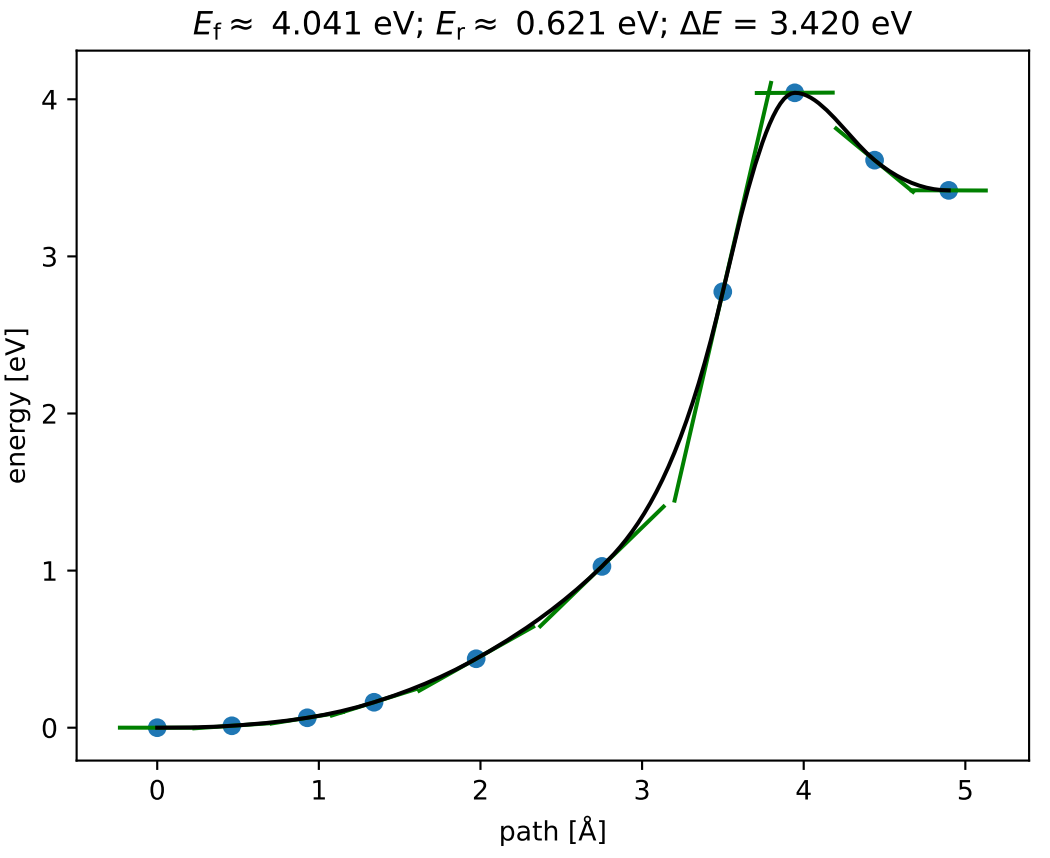
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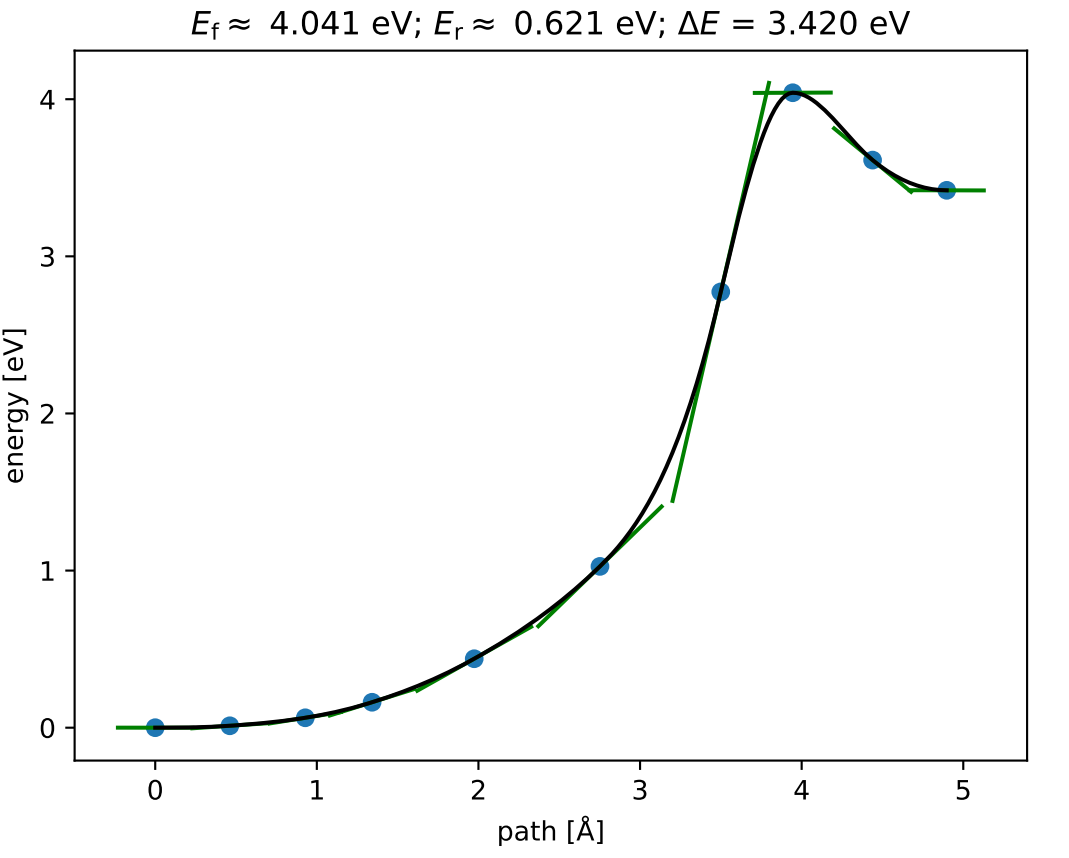
$E_f \approx$ 4.041 eV; $E_r \approx$ 0.621 eV; ΔE = 3.420 eV
energy [eV]
path [Å]
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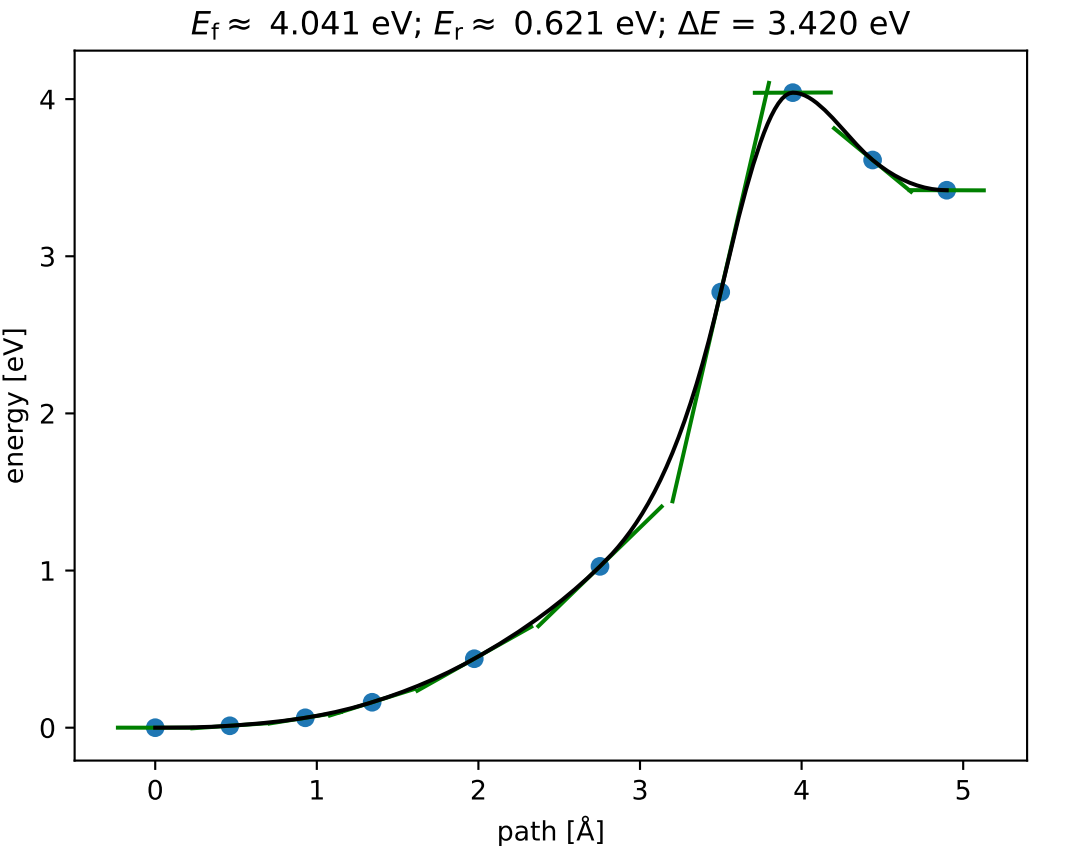
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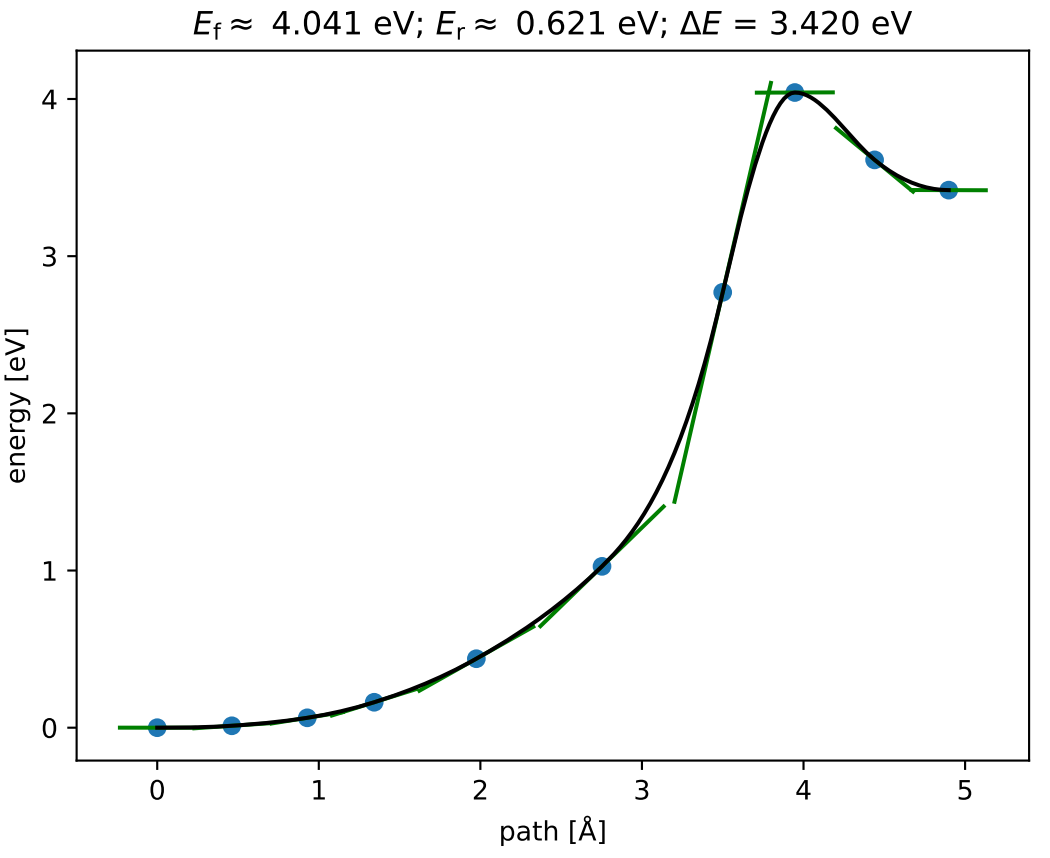
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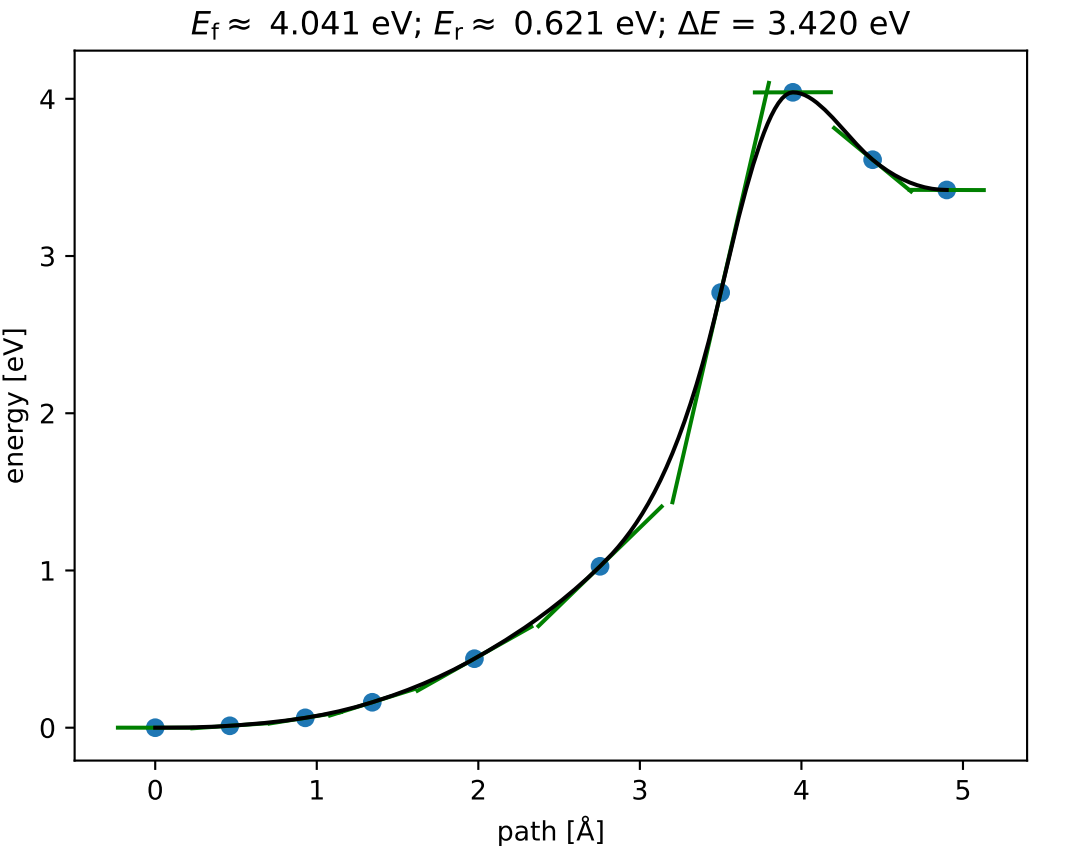
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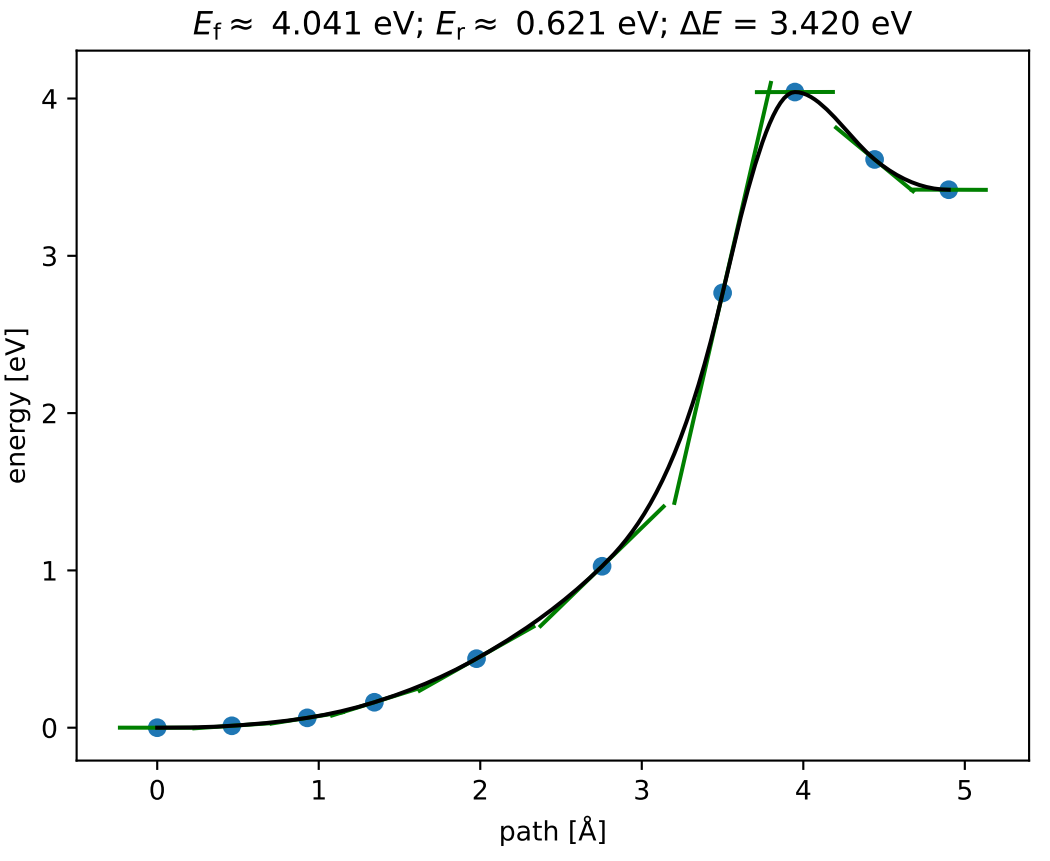
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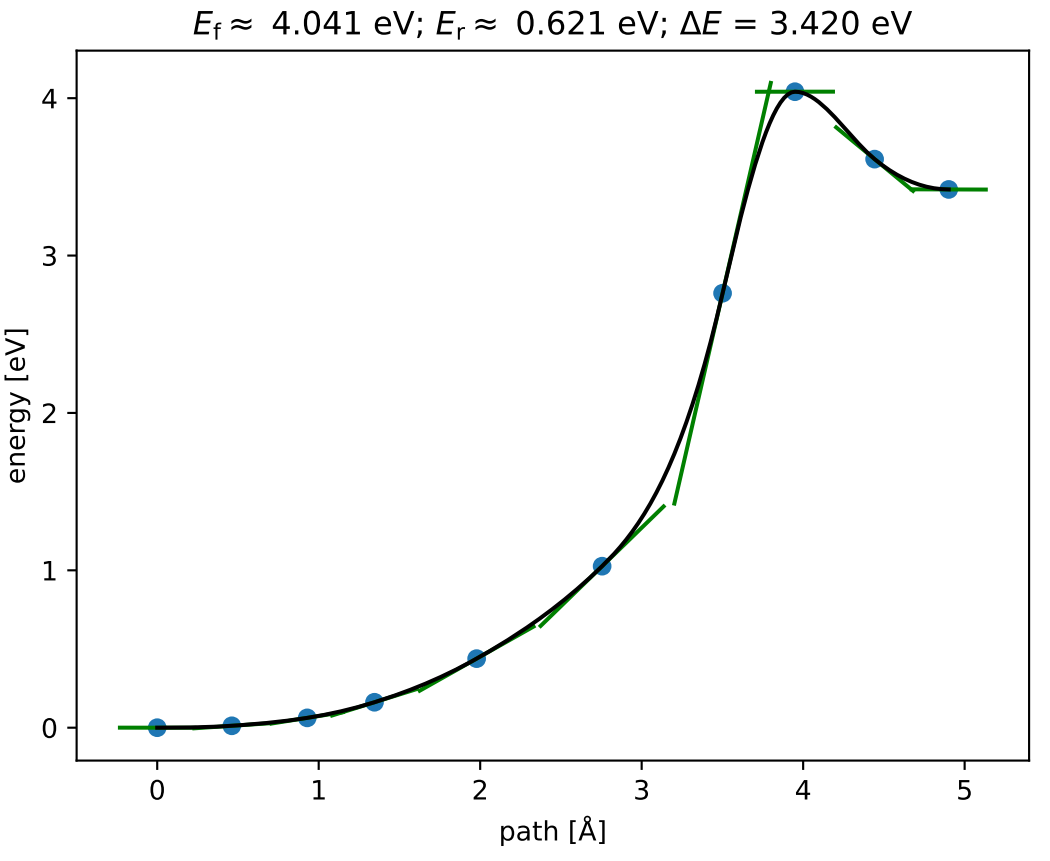
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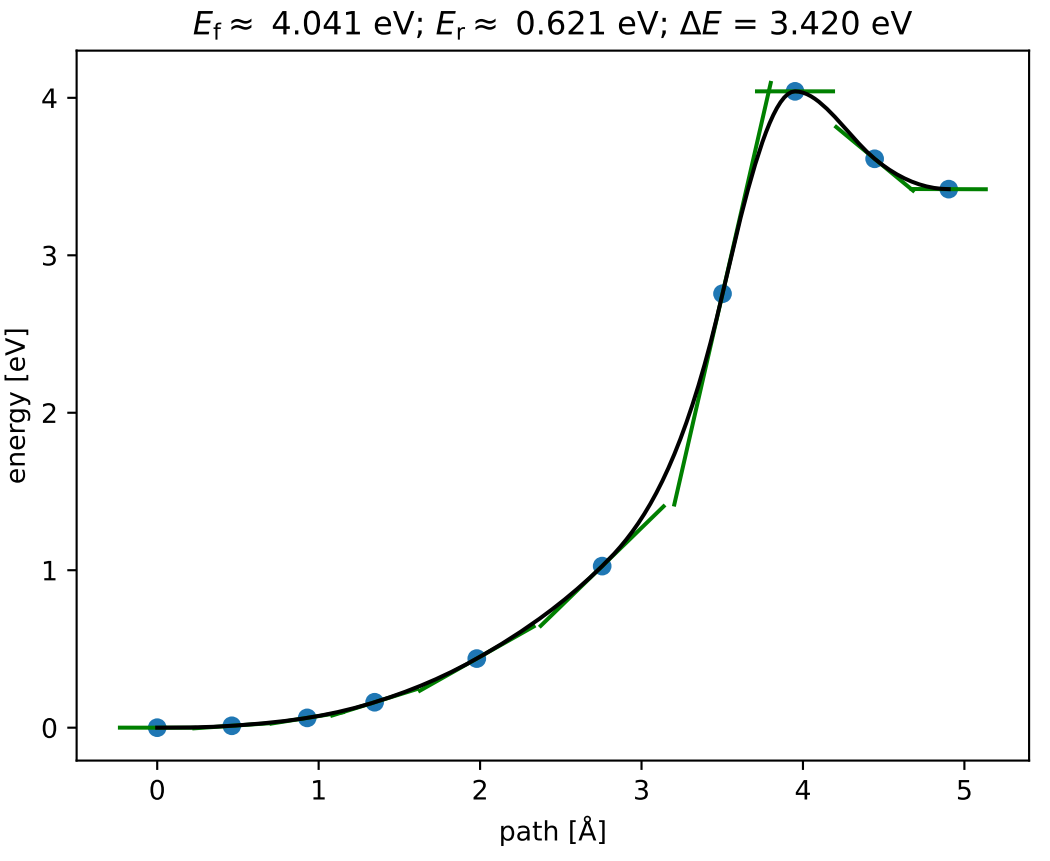
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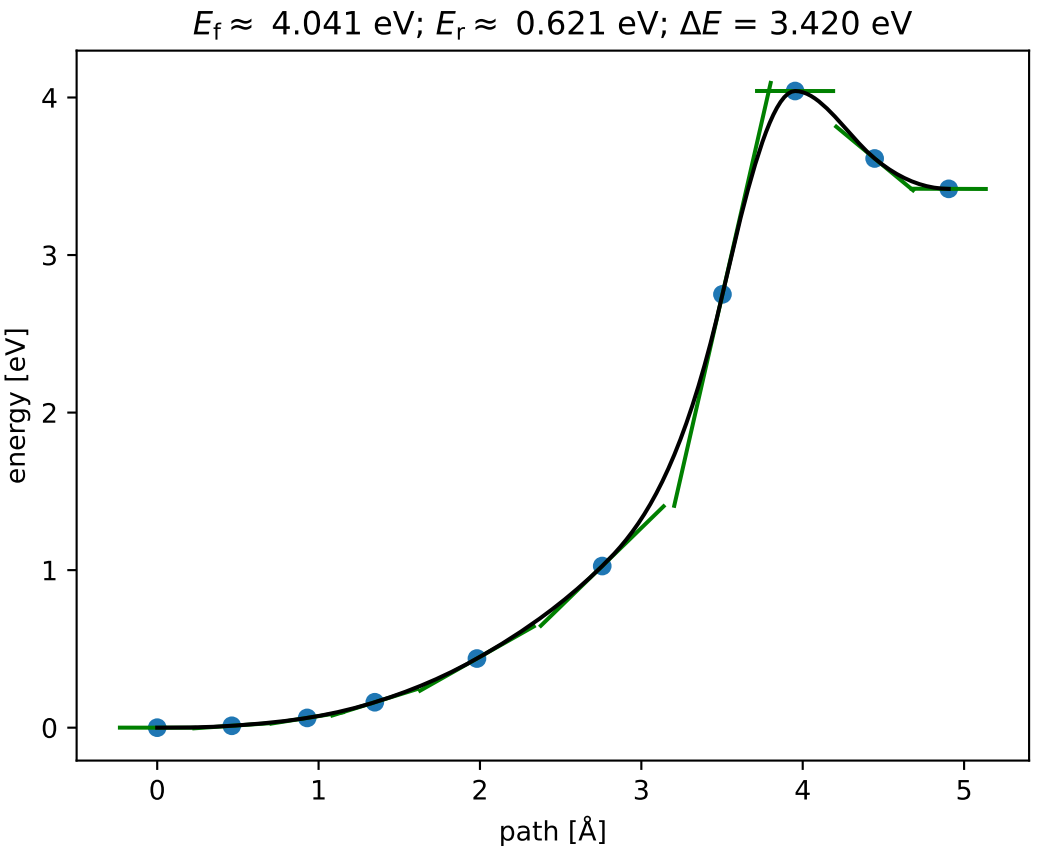
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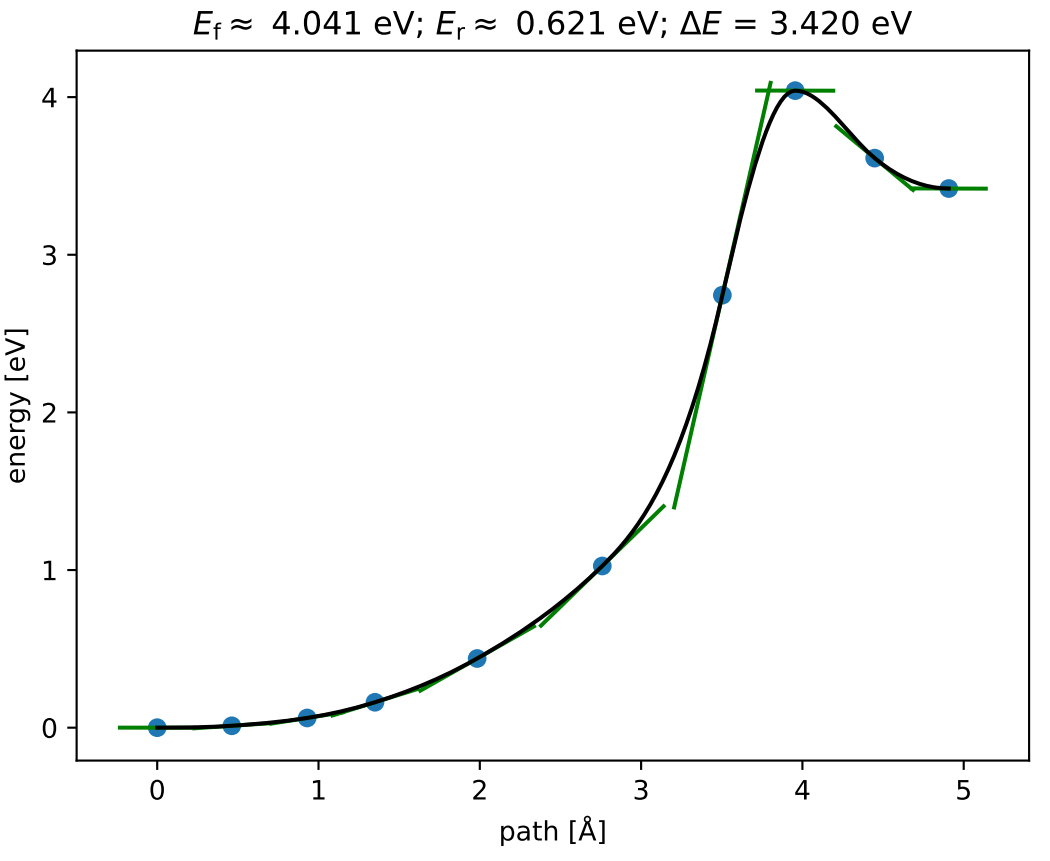
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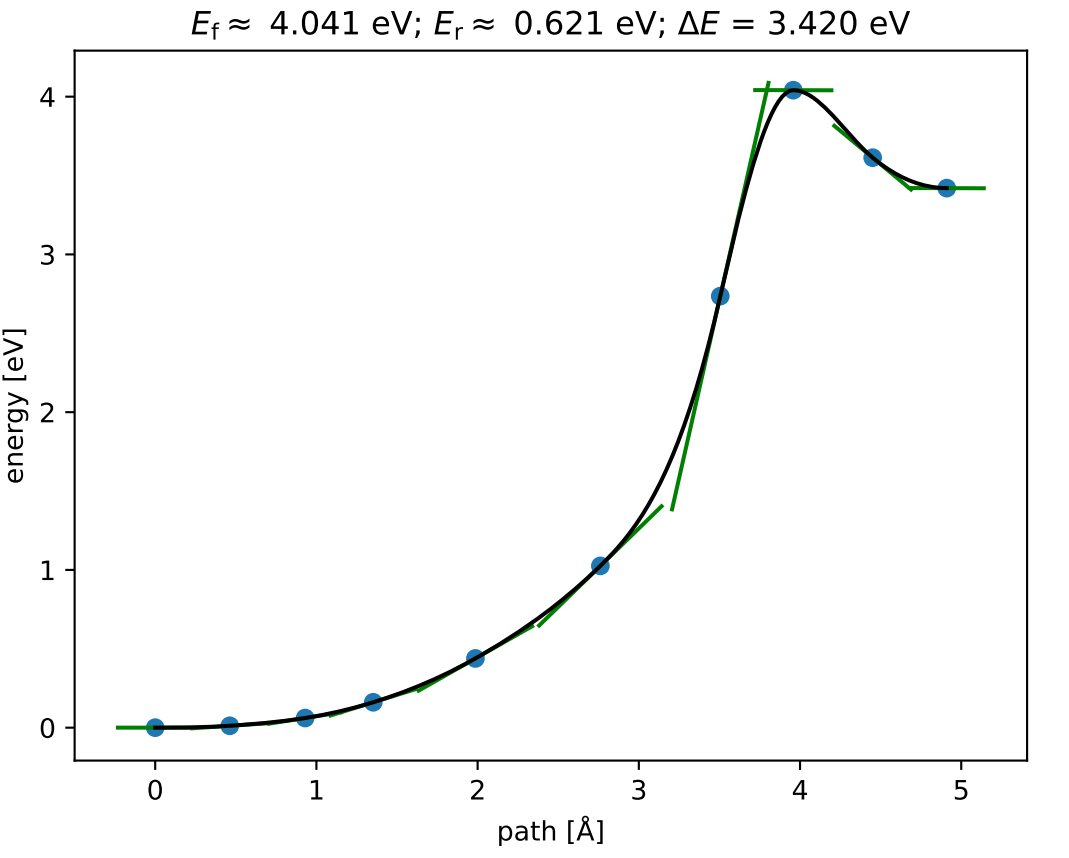
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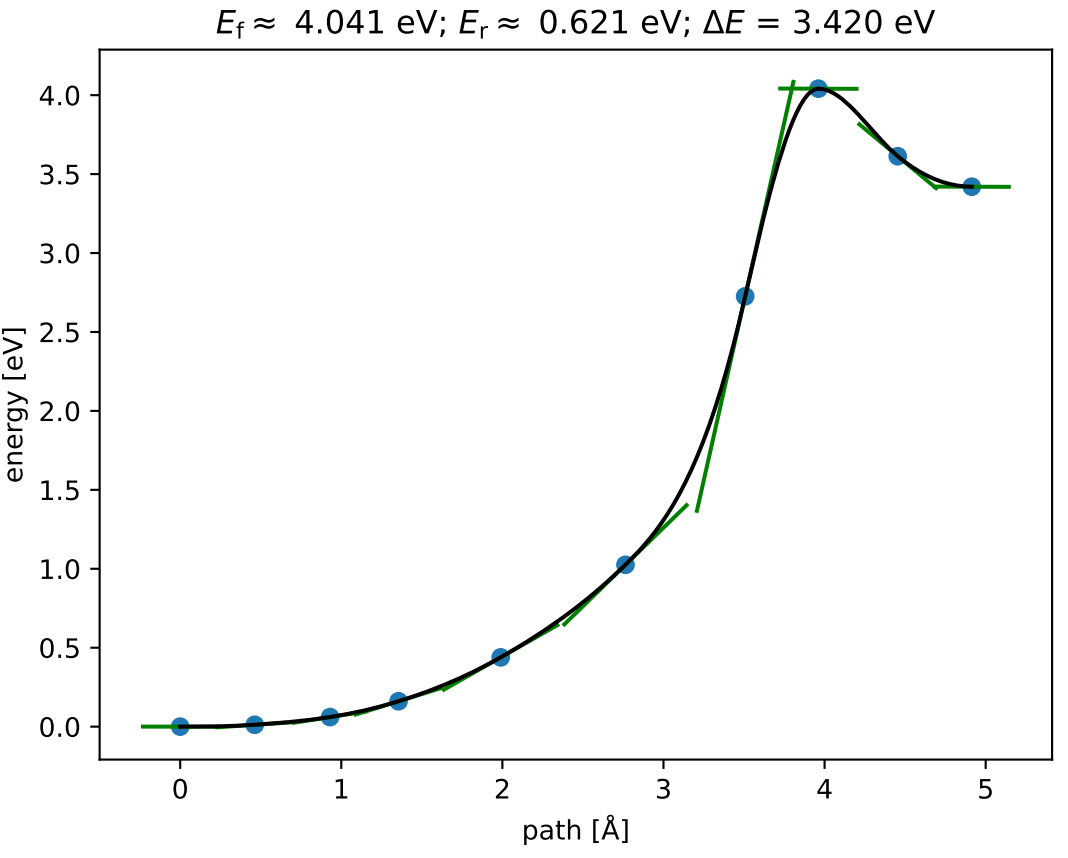
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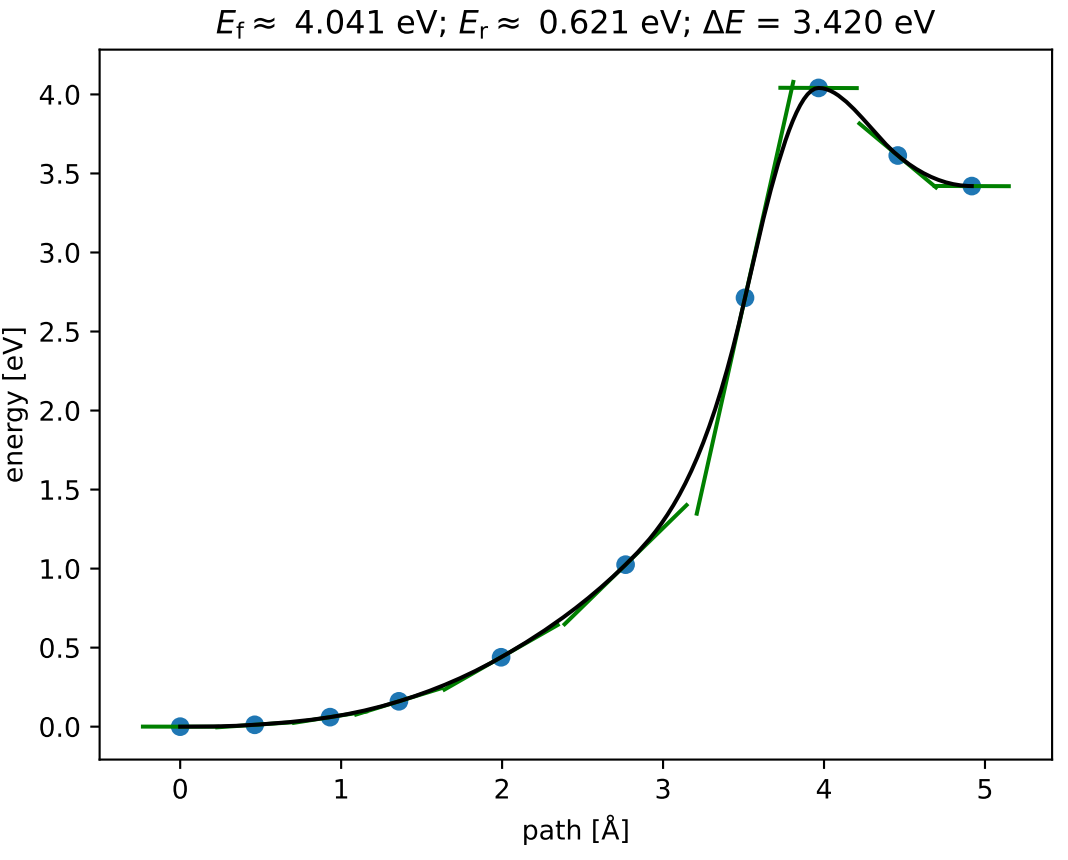
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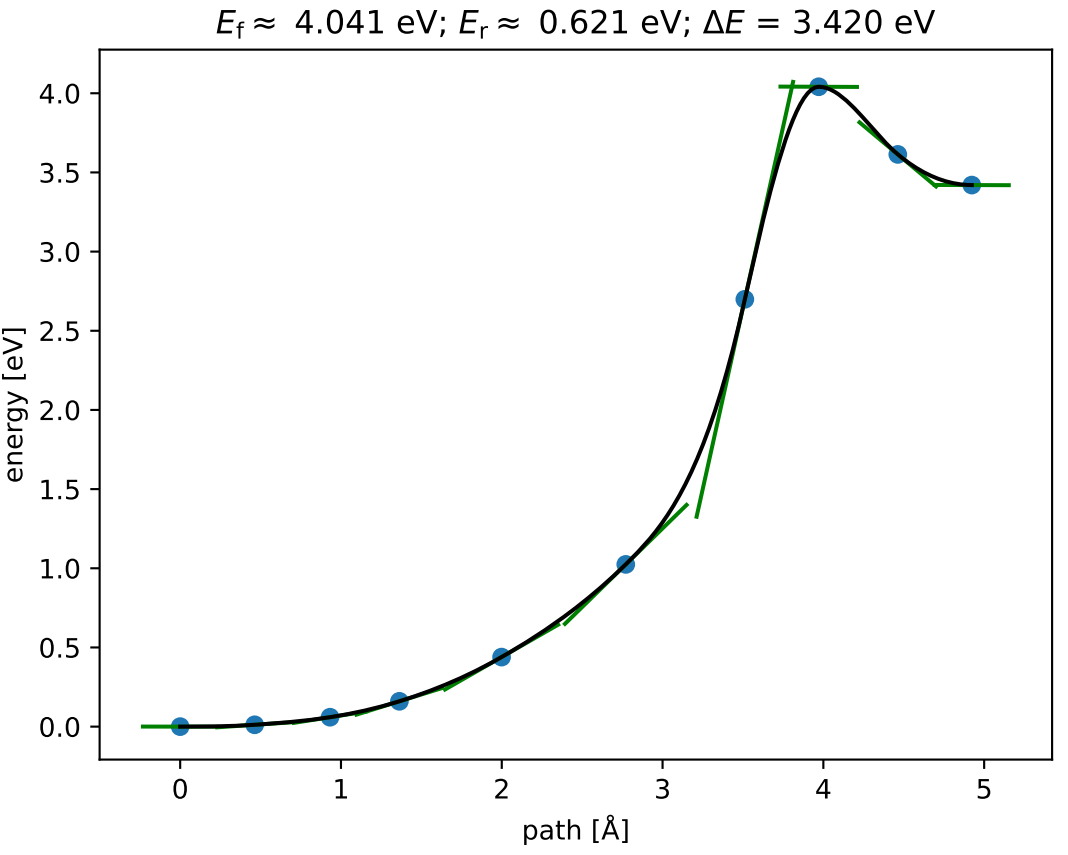
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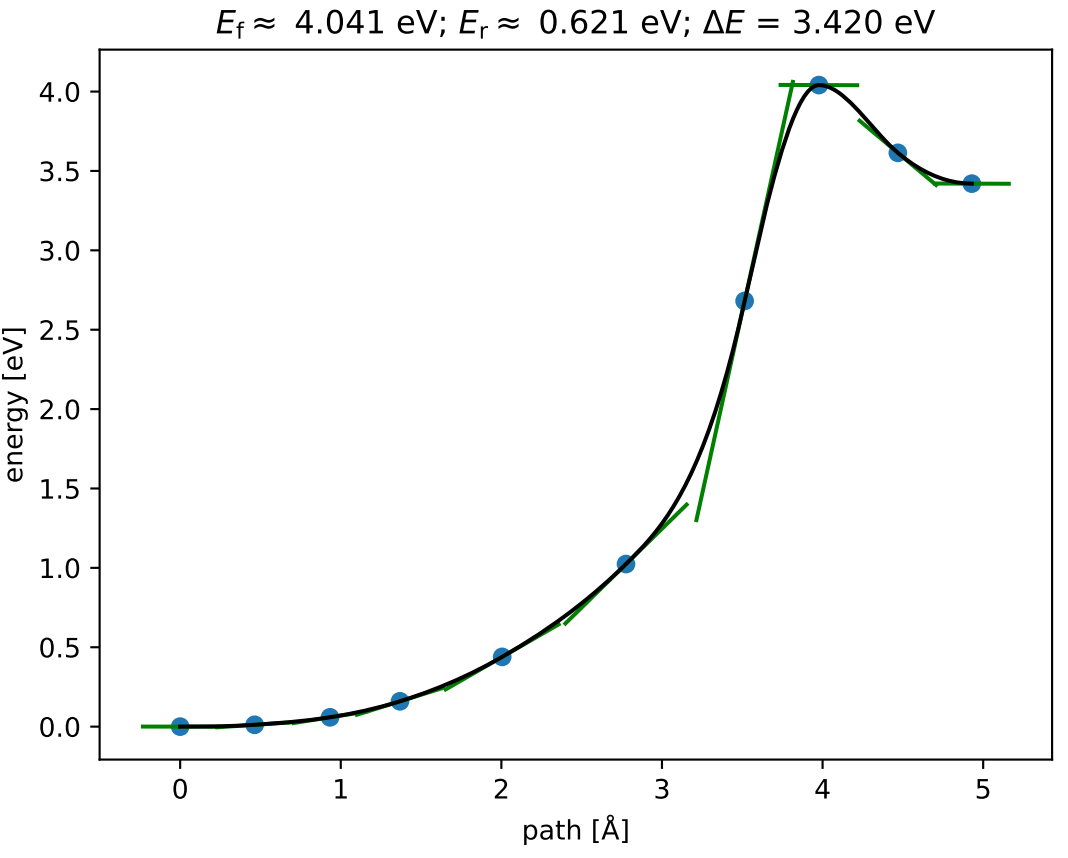
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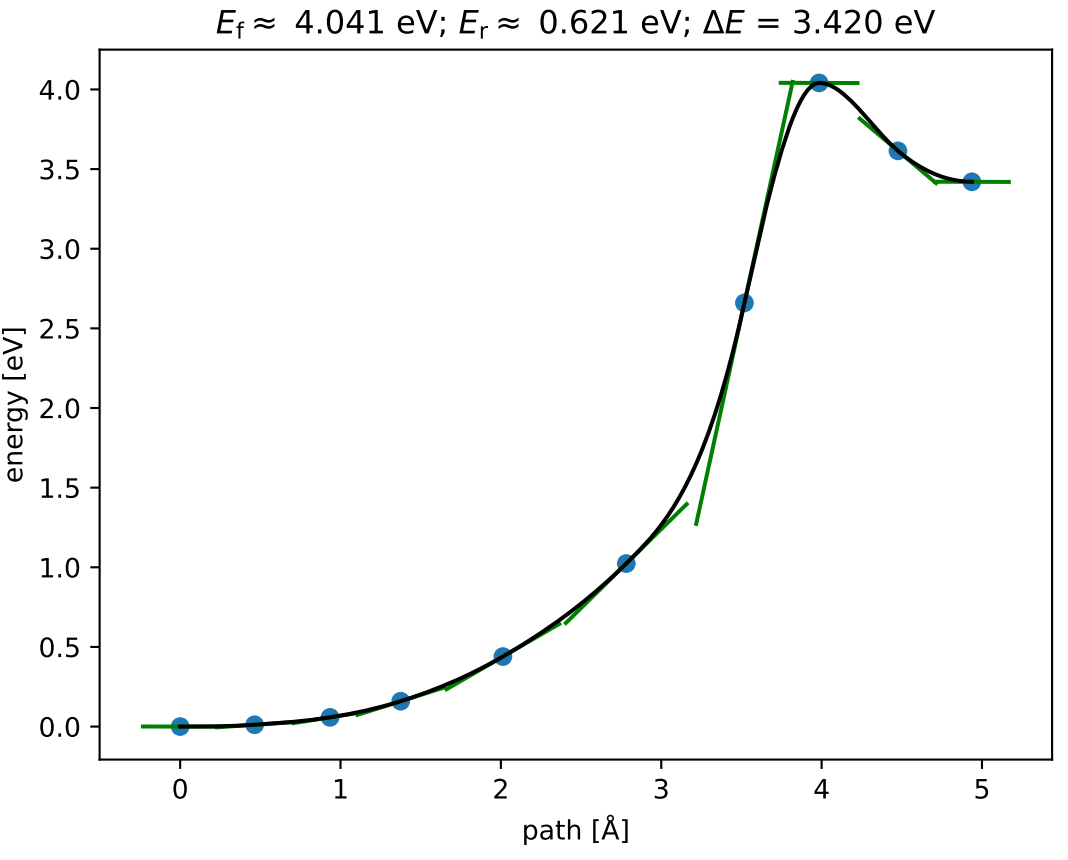
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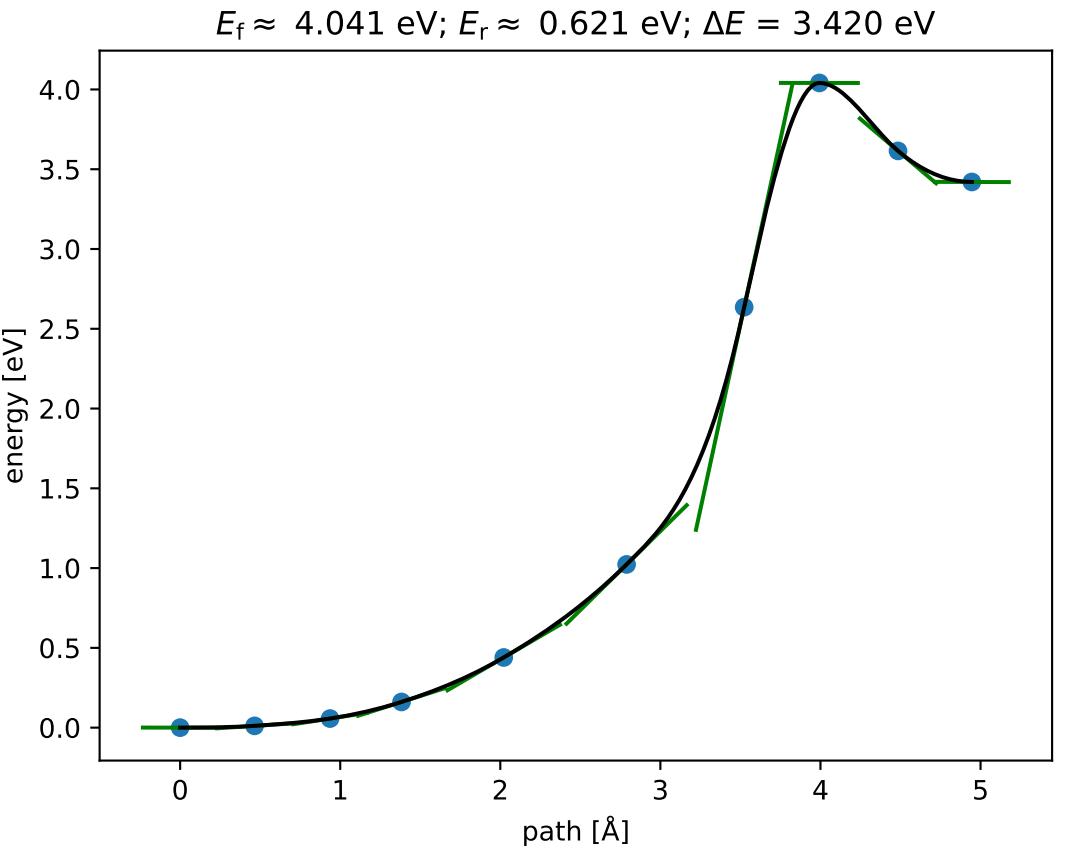
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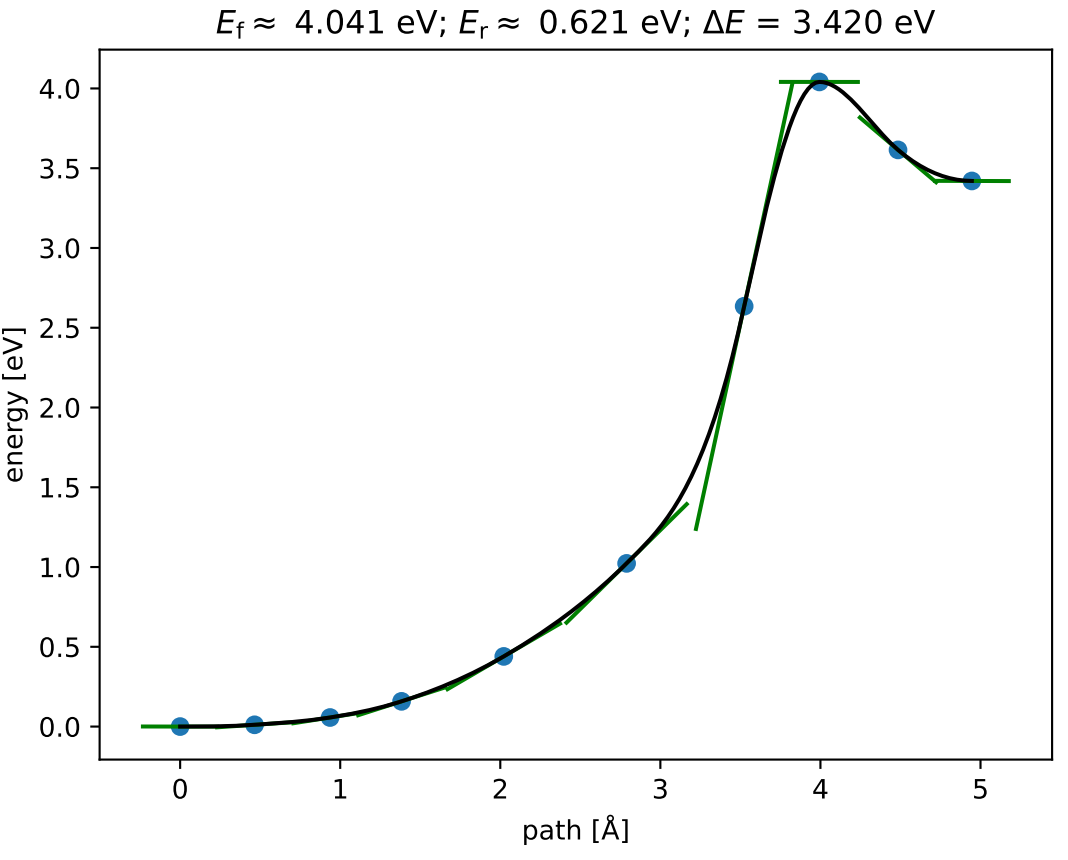
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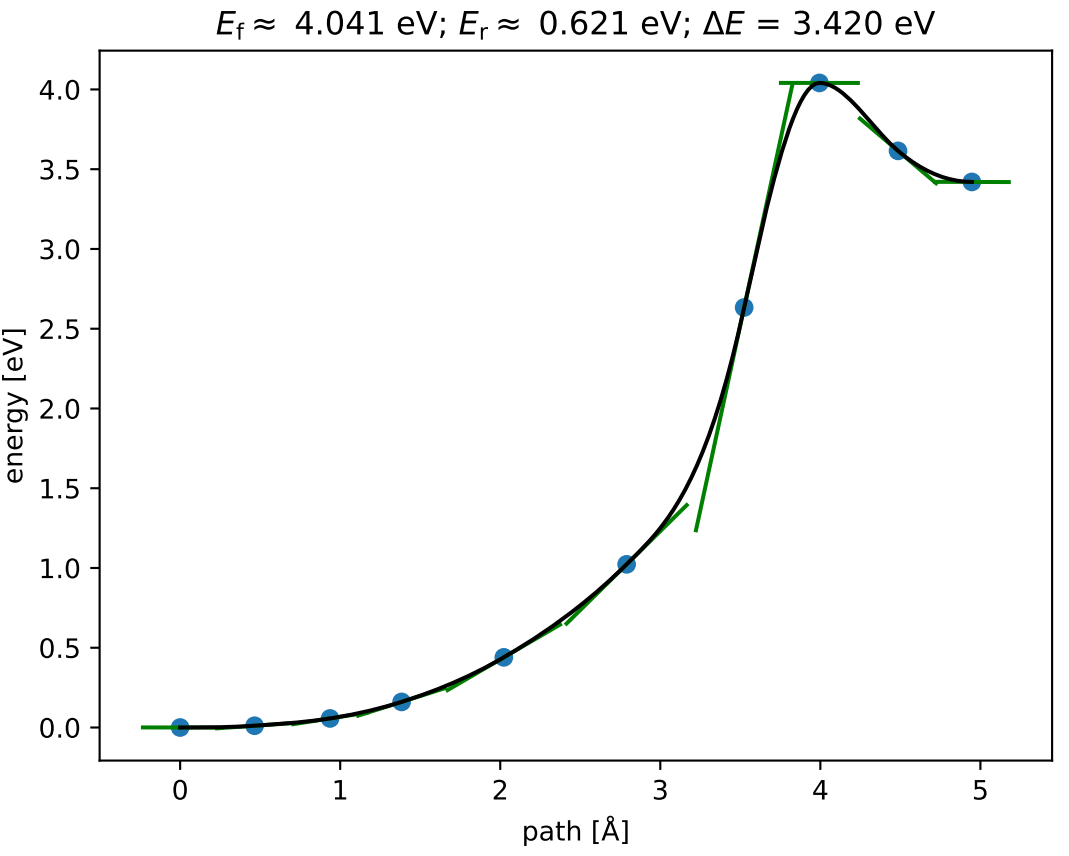
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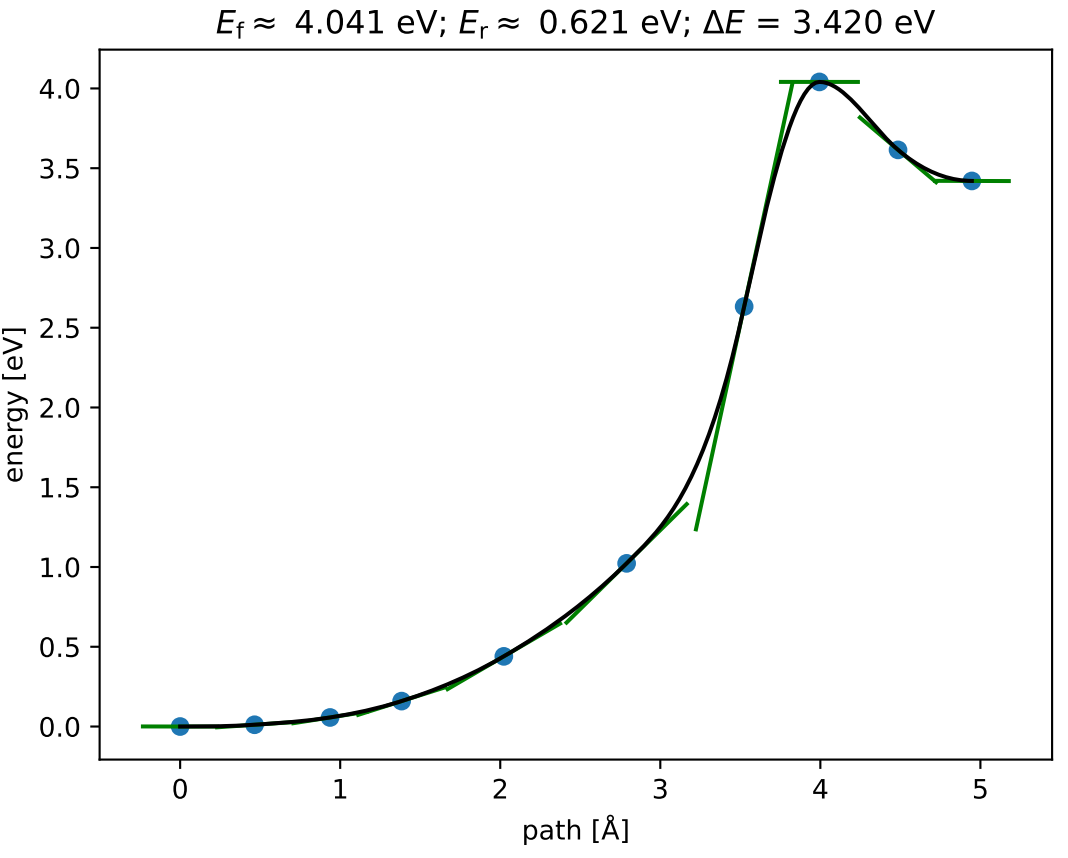
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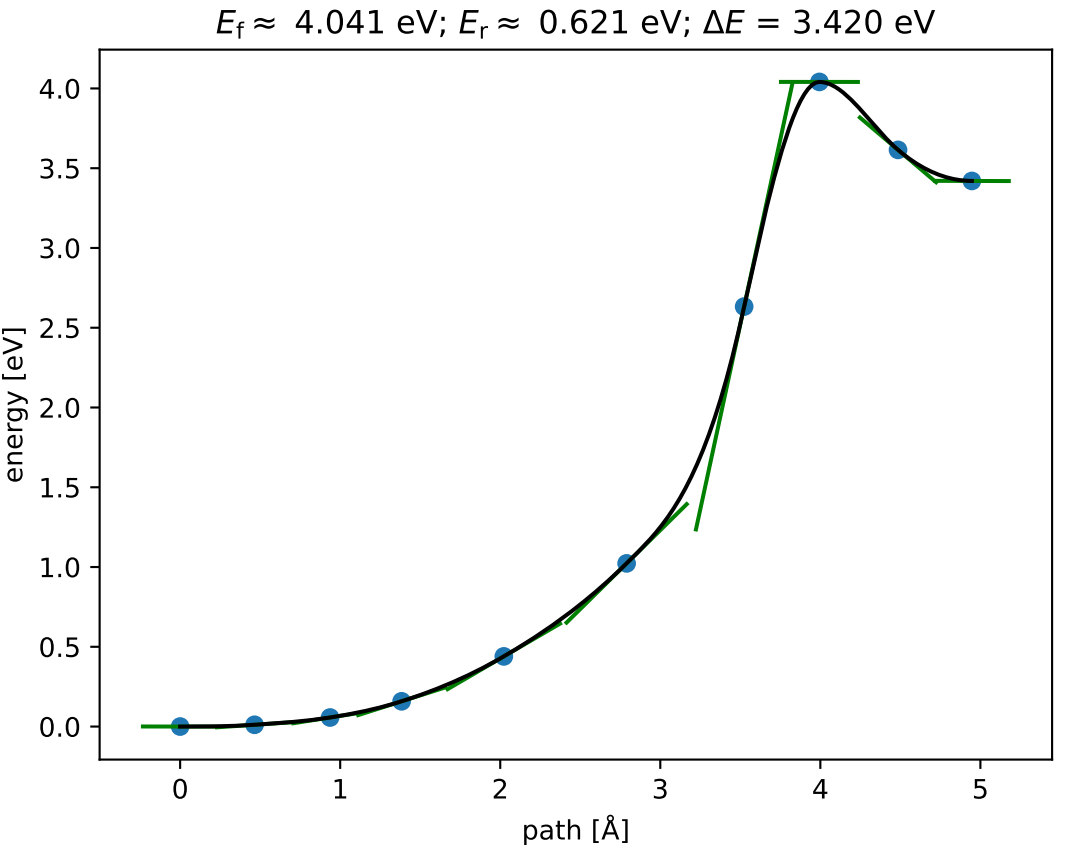
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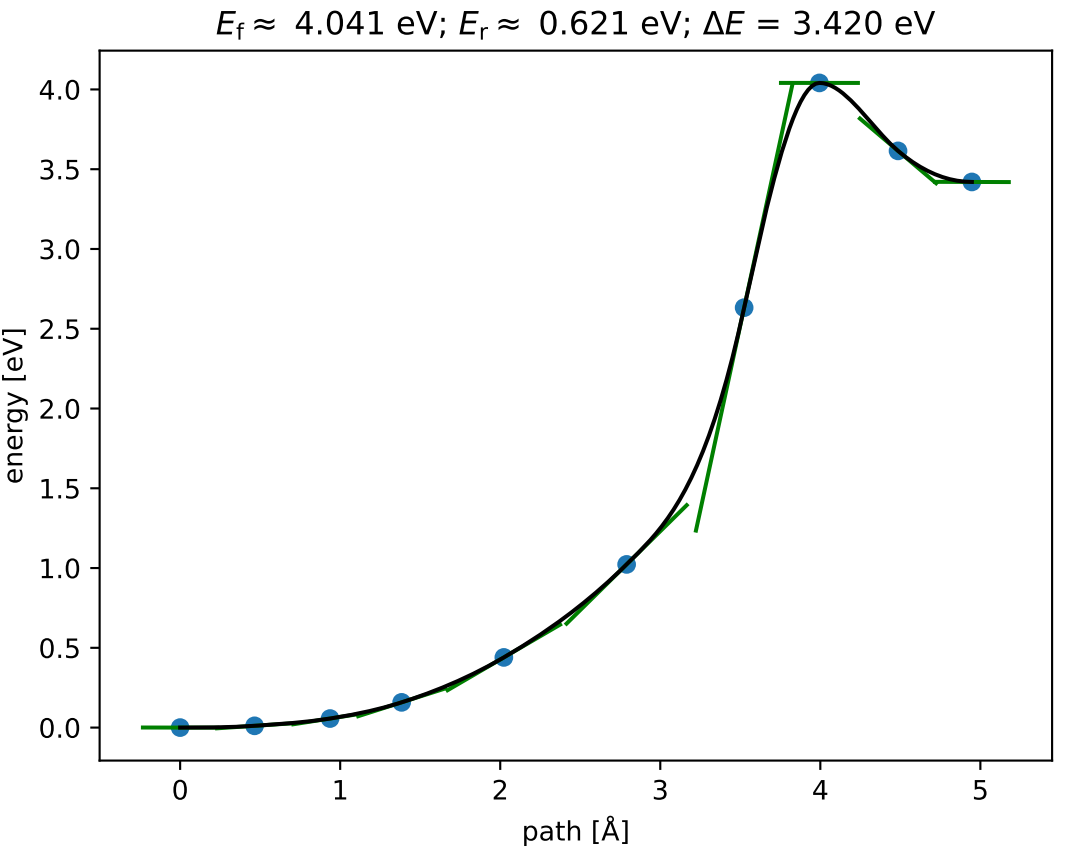
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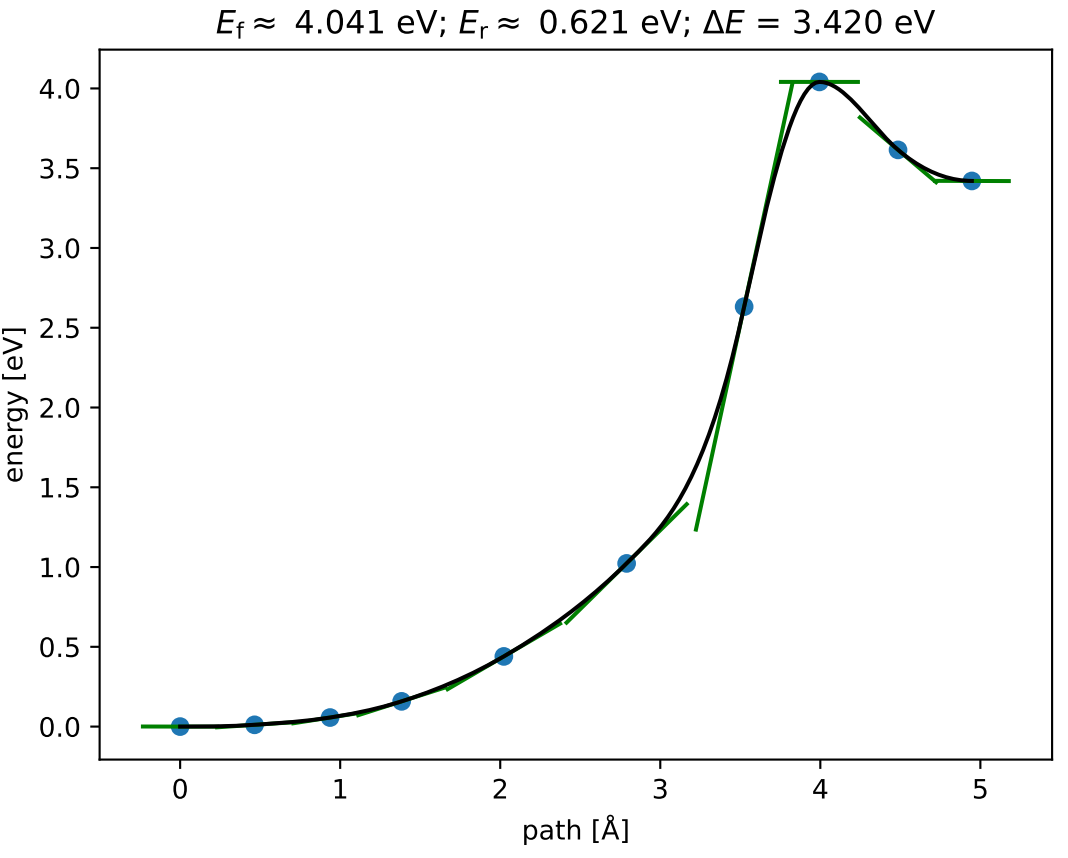
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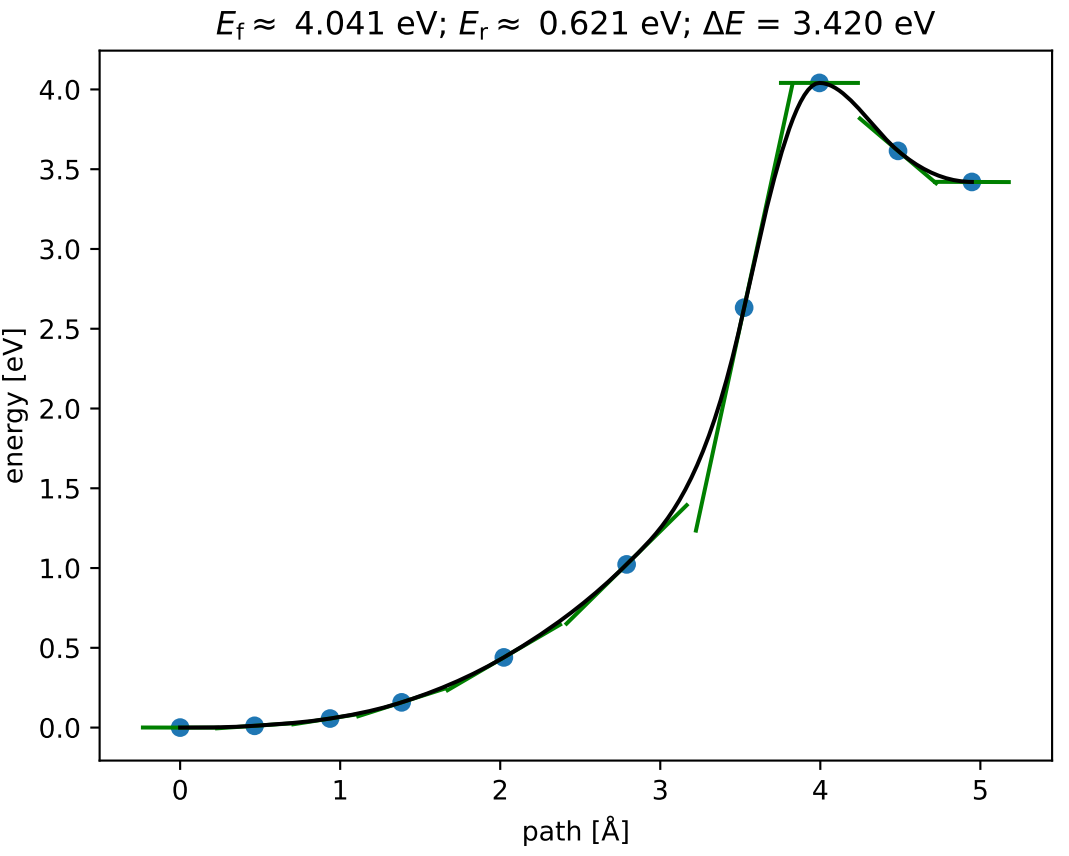
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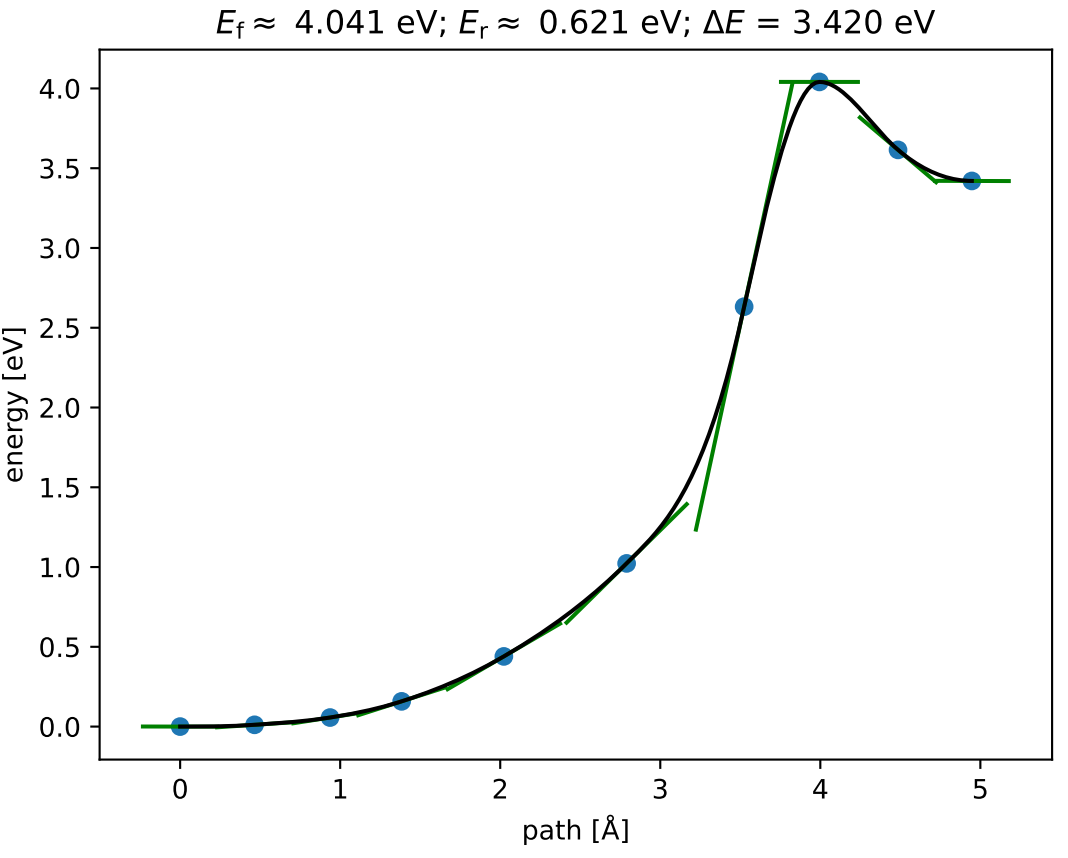
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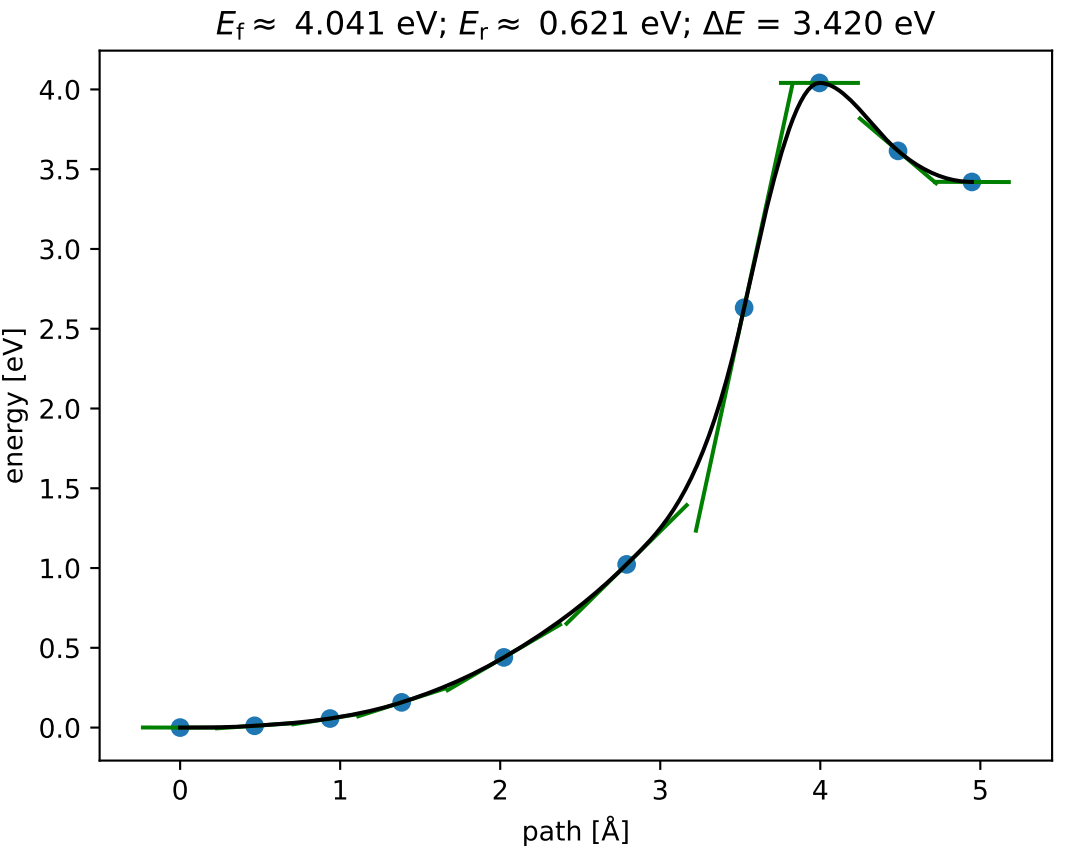
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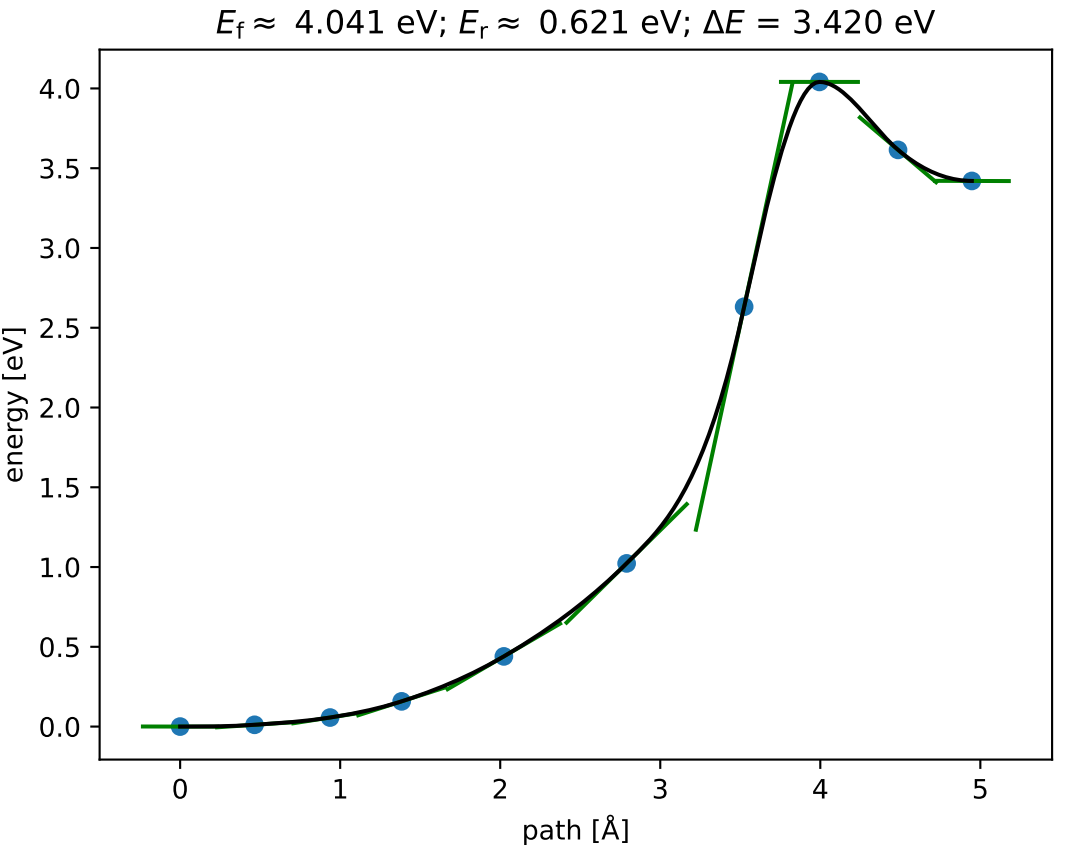
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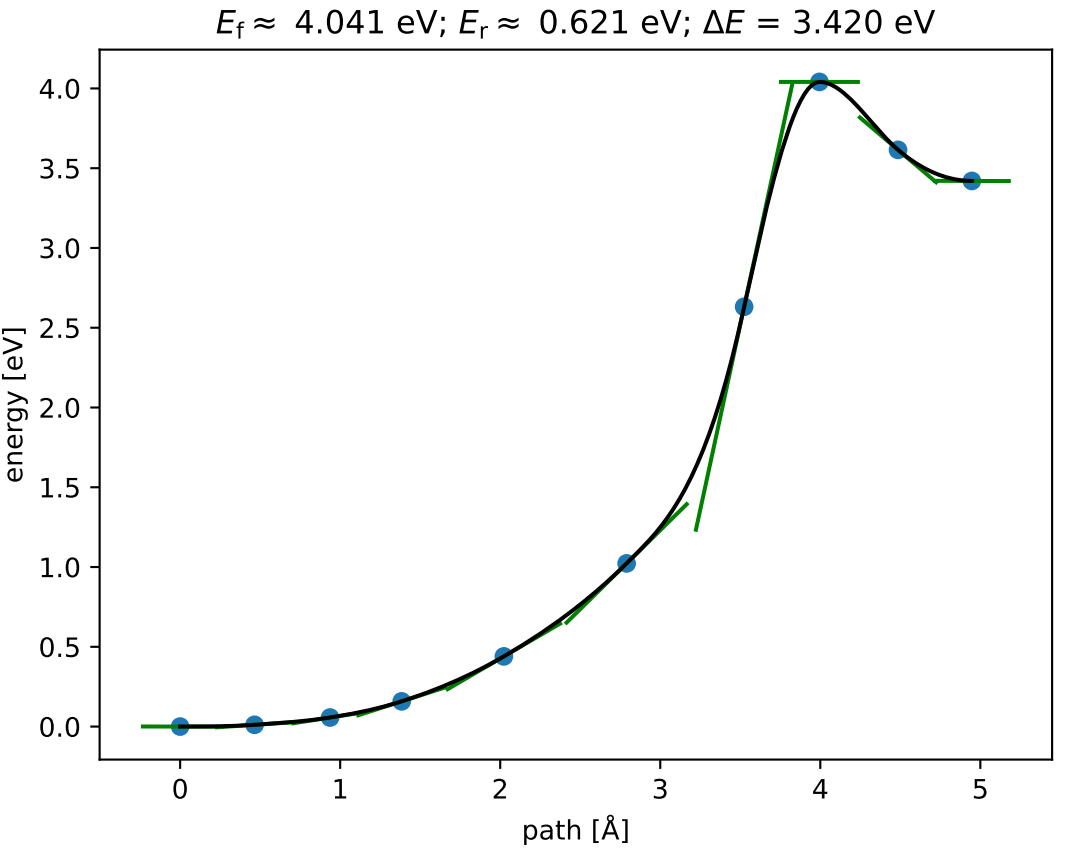
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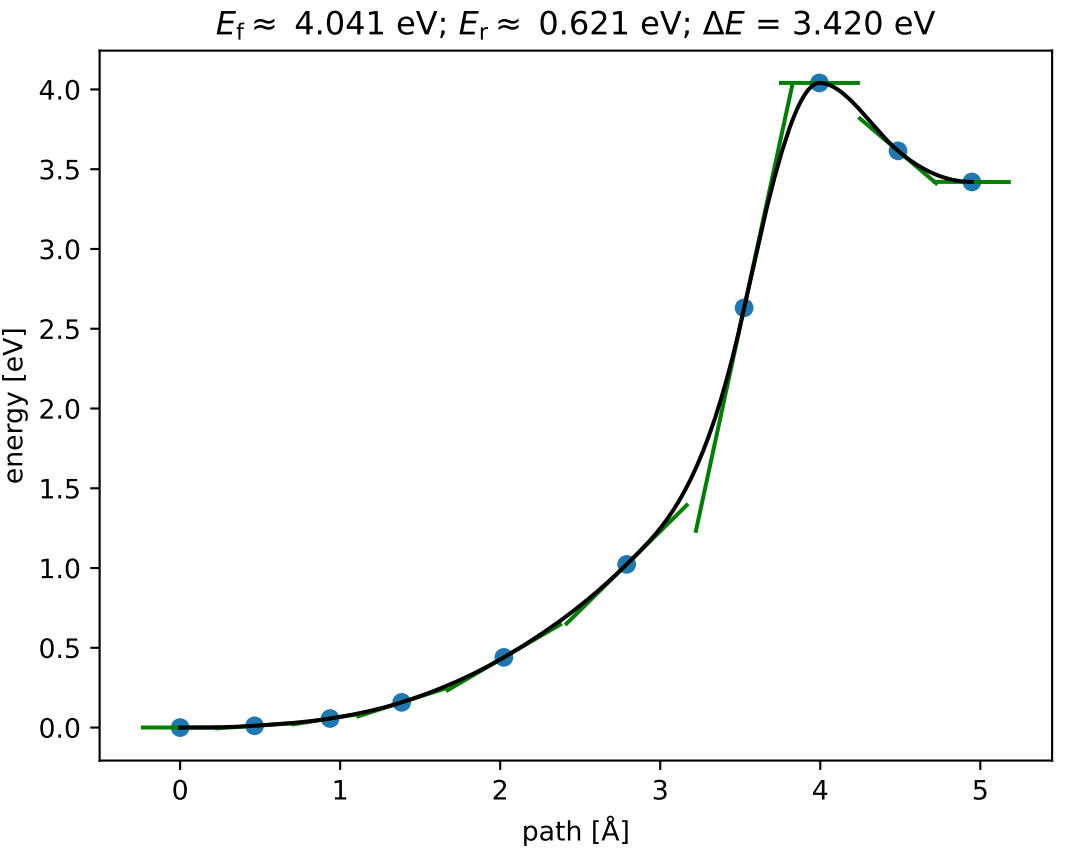
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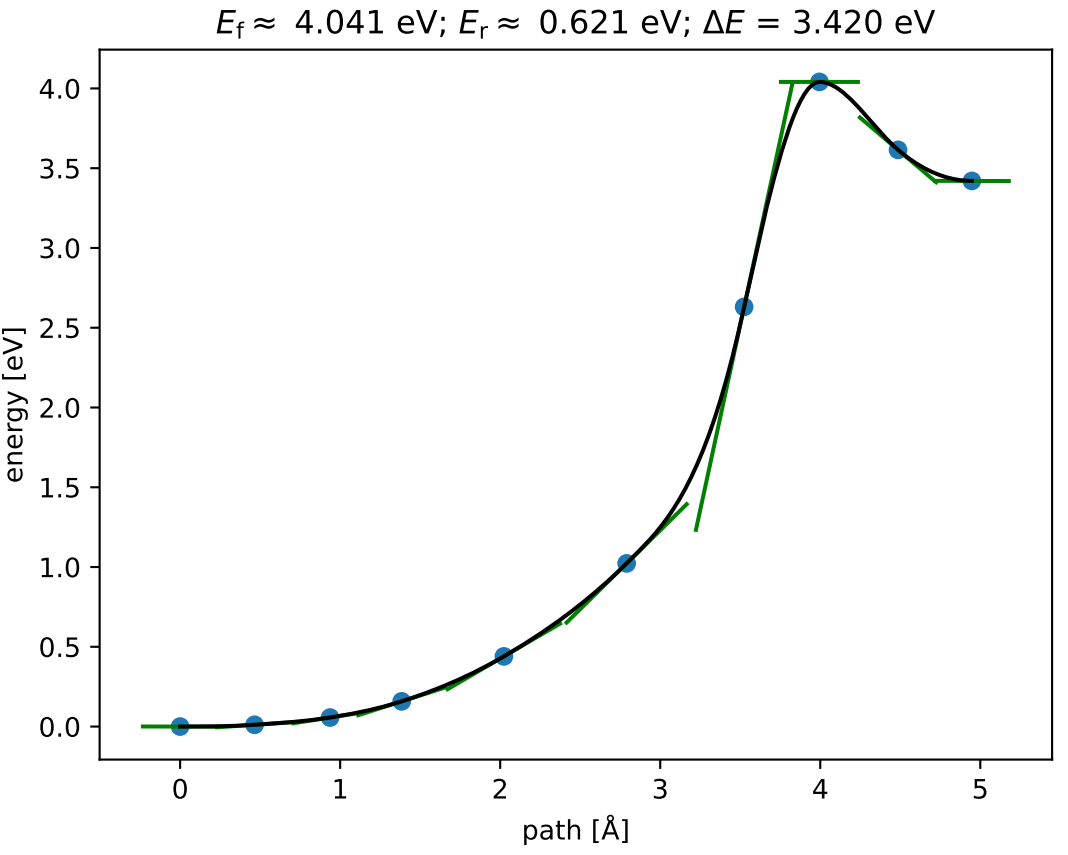
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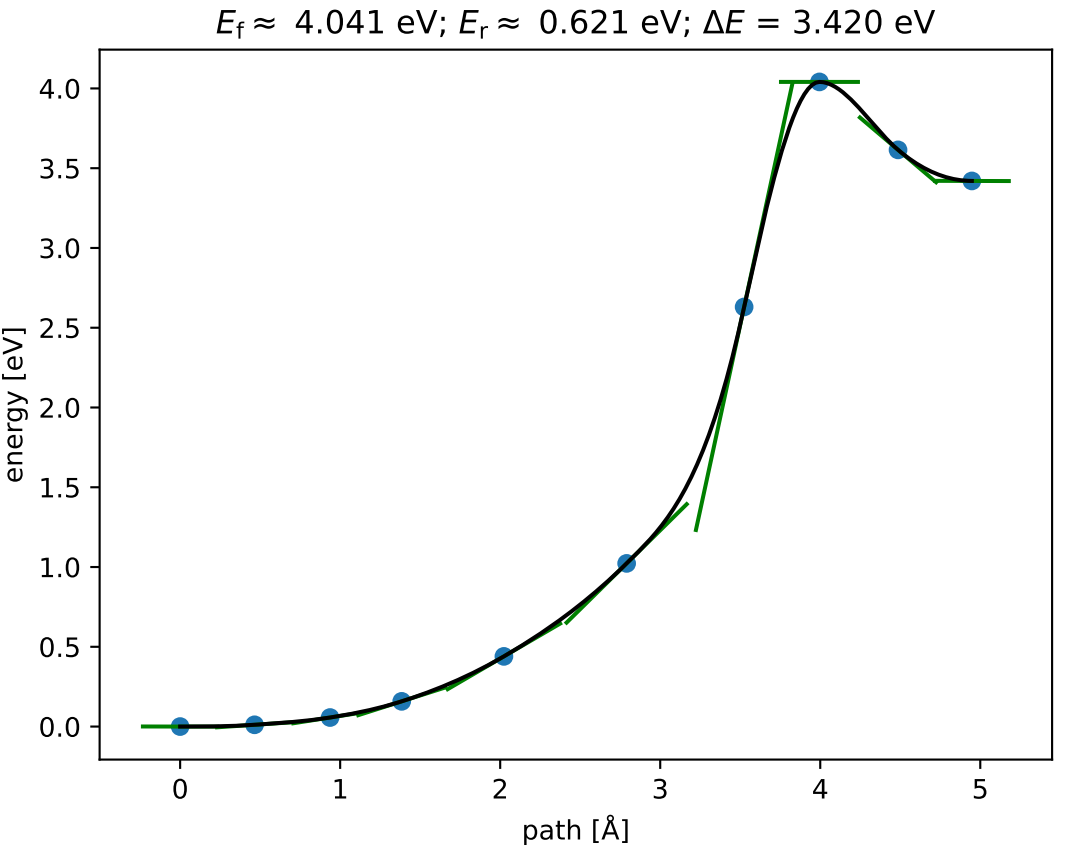
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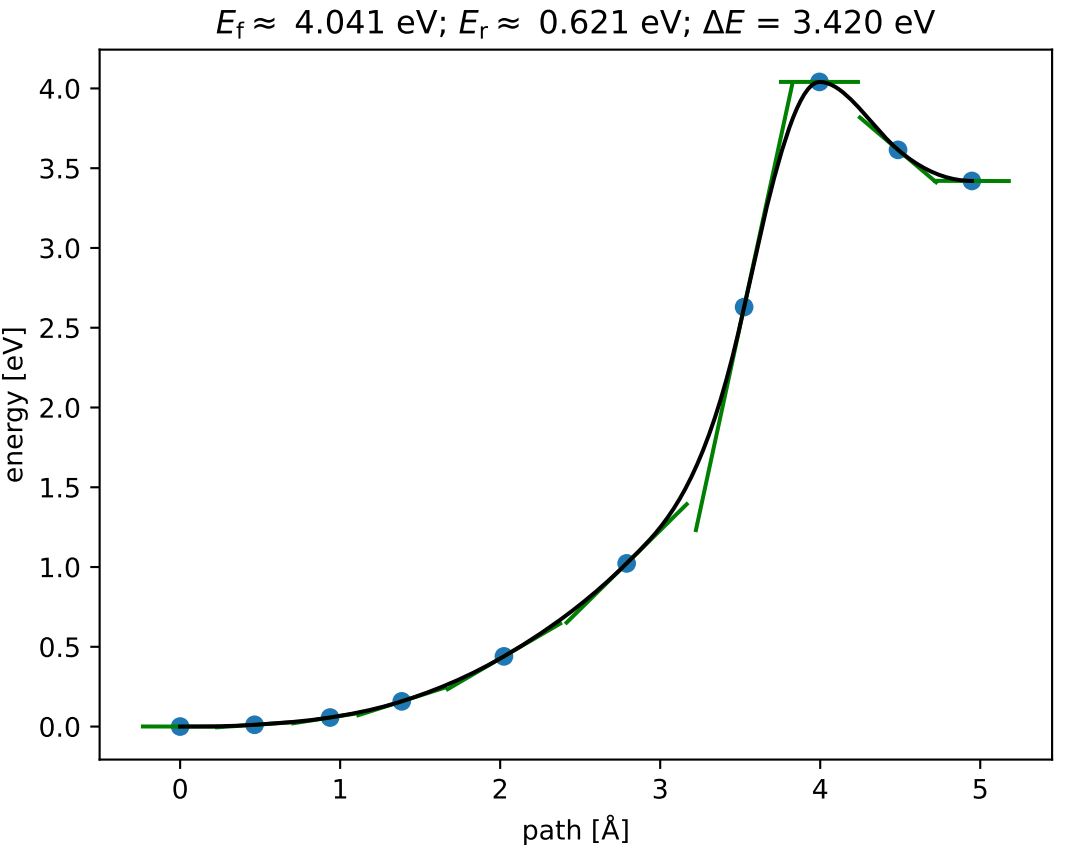
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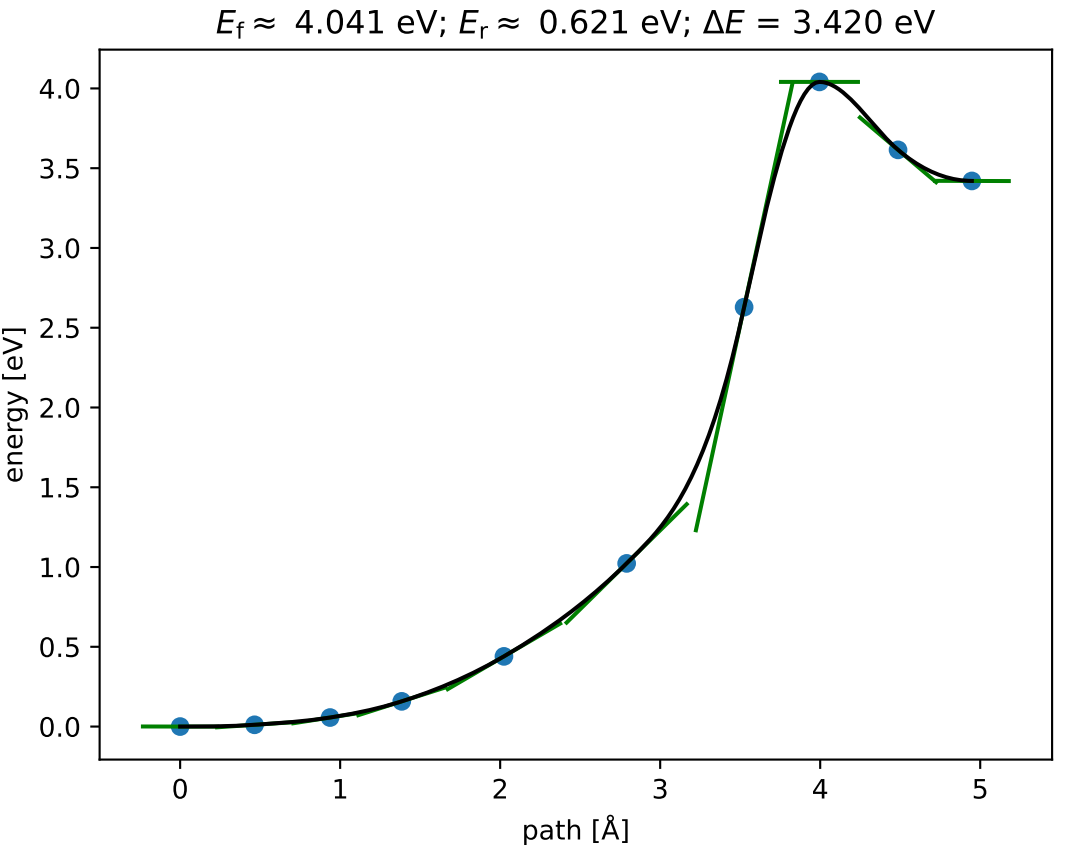
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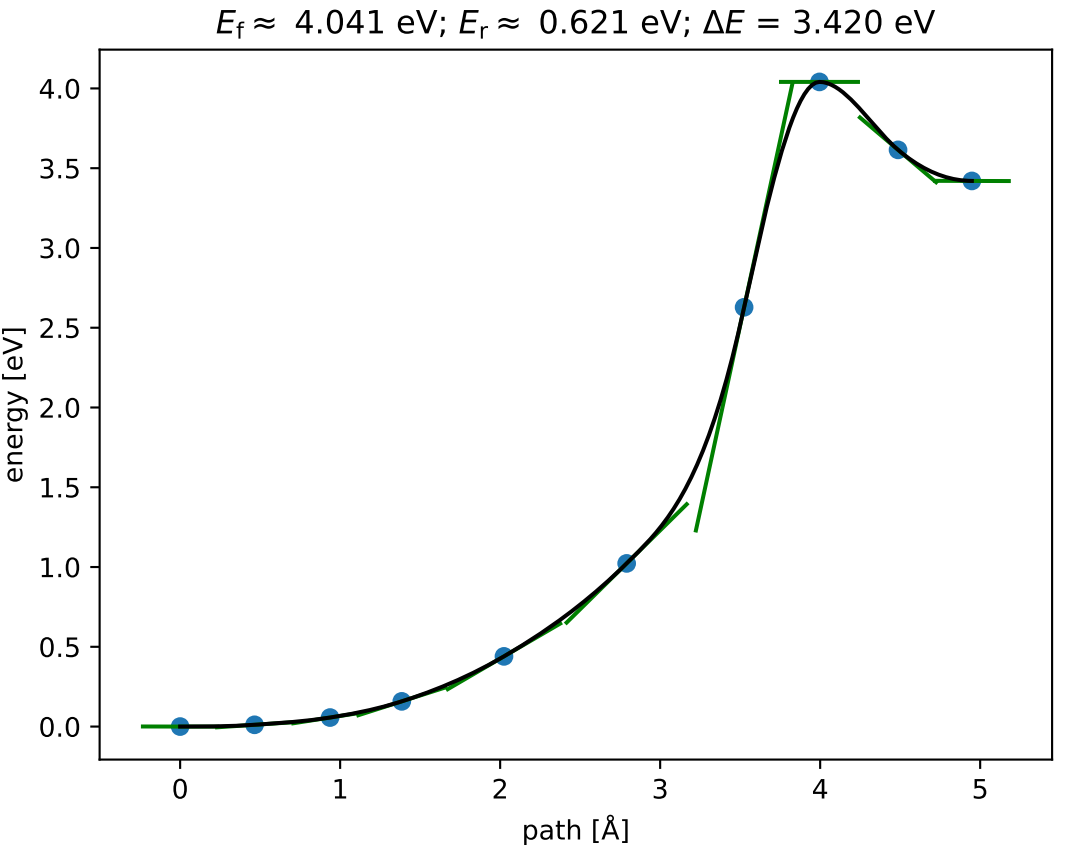
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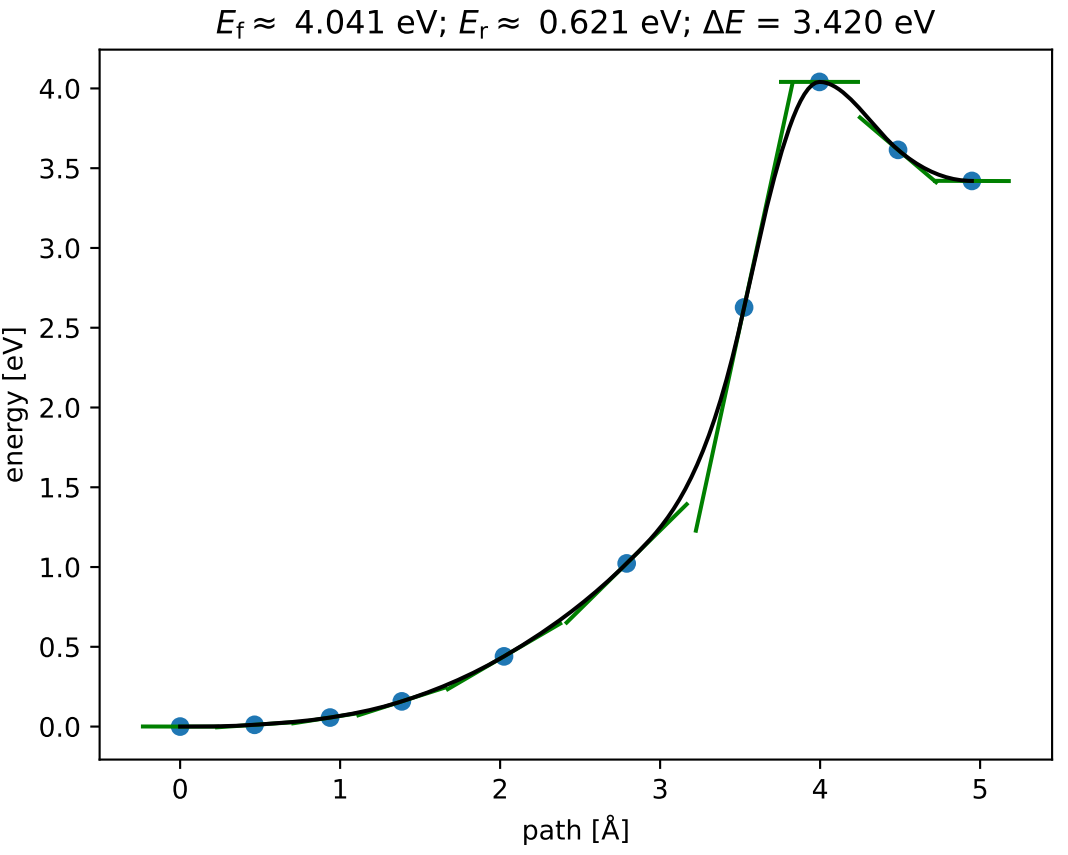
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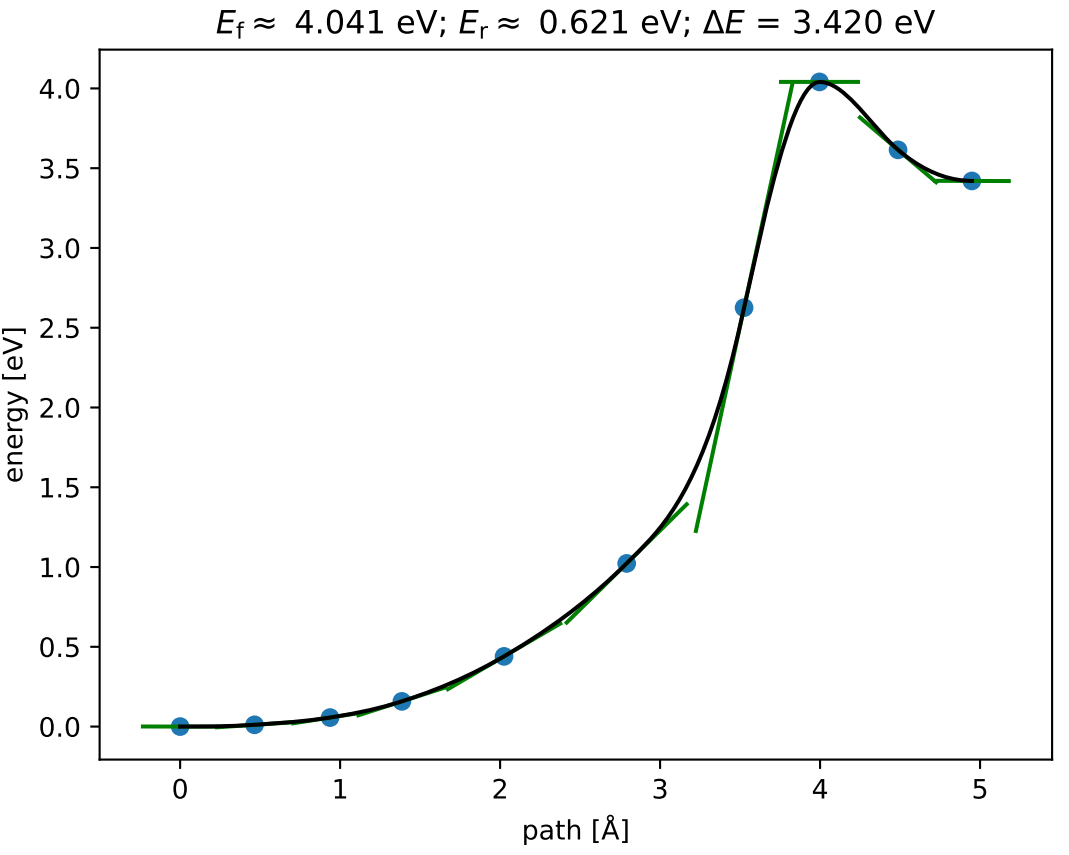
$E_f \approx$ 4.041 eV; $E_r \approx$ 0.621 eV; ΔE = 3.420 eV
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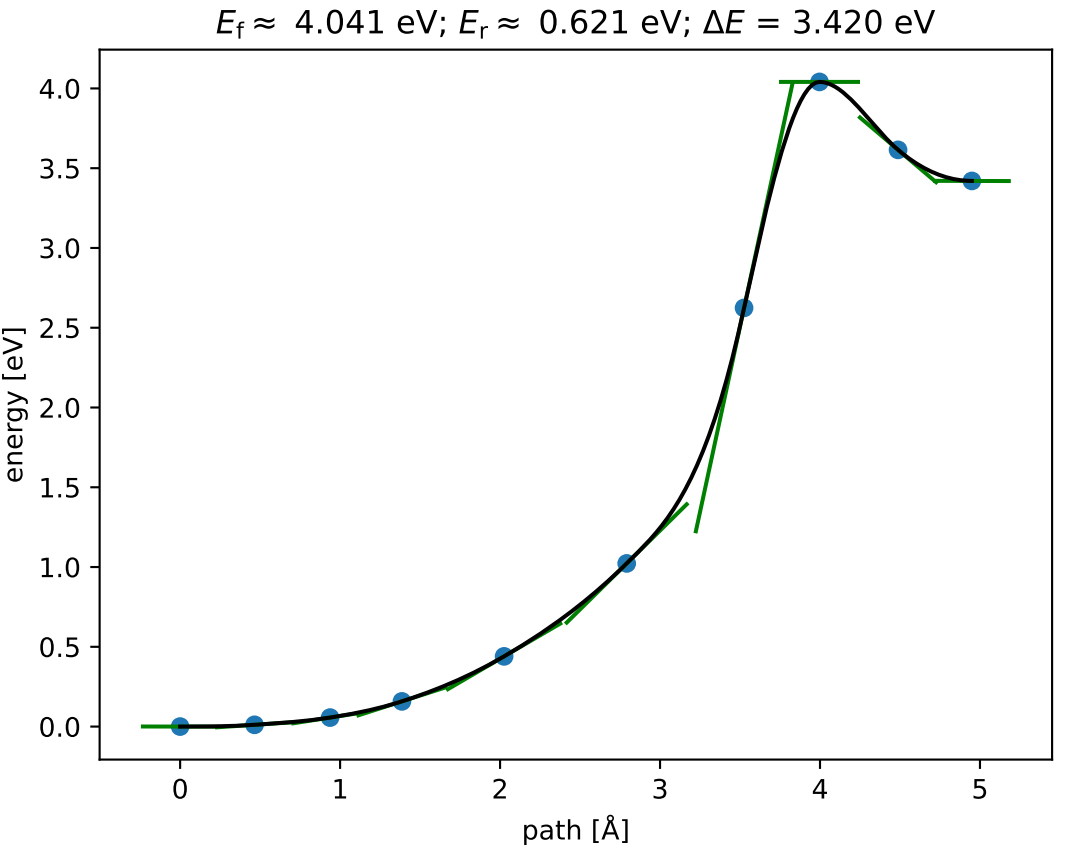
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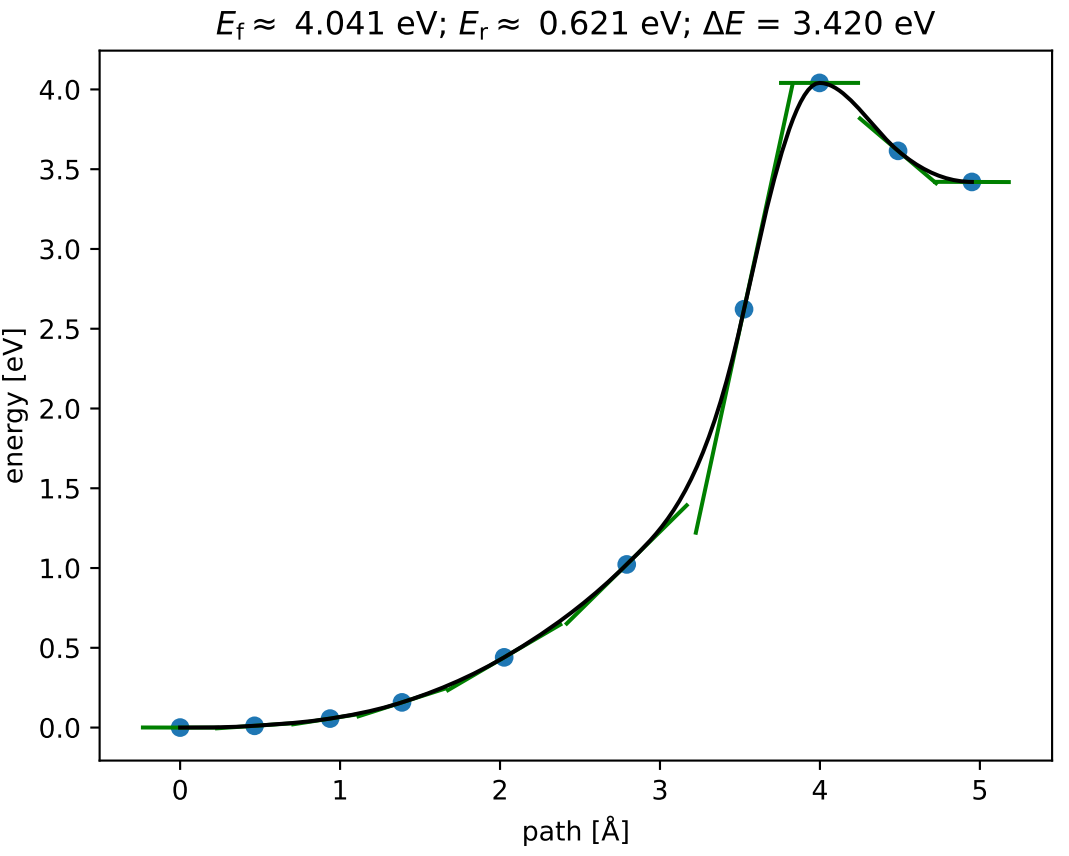
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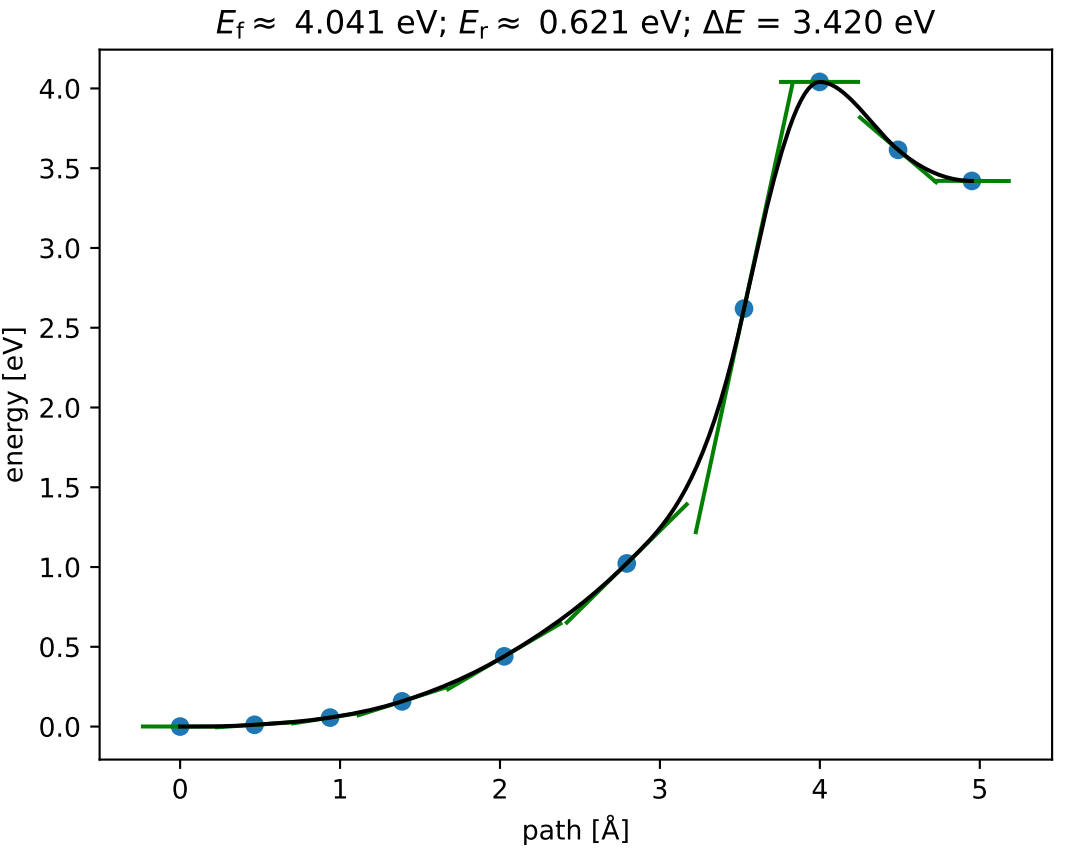
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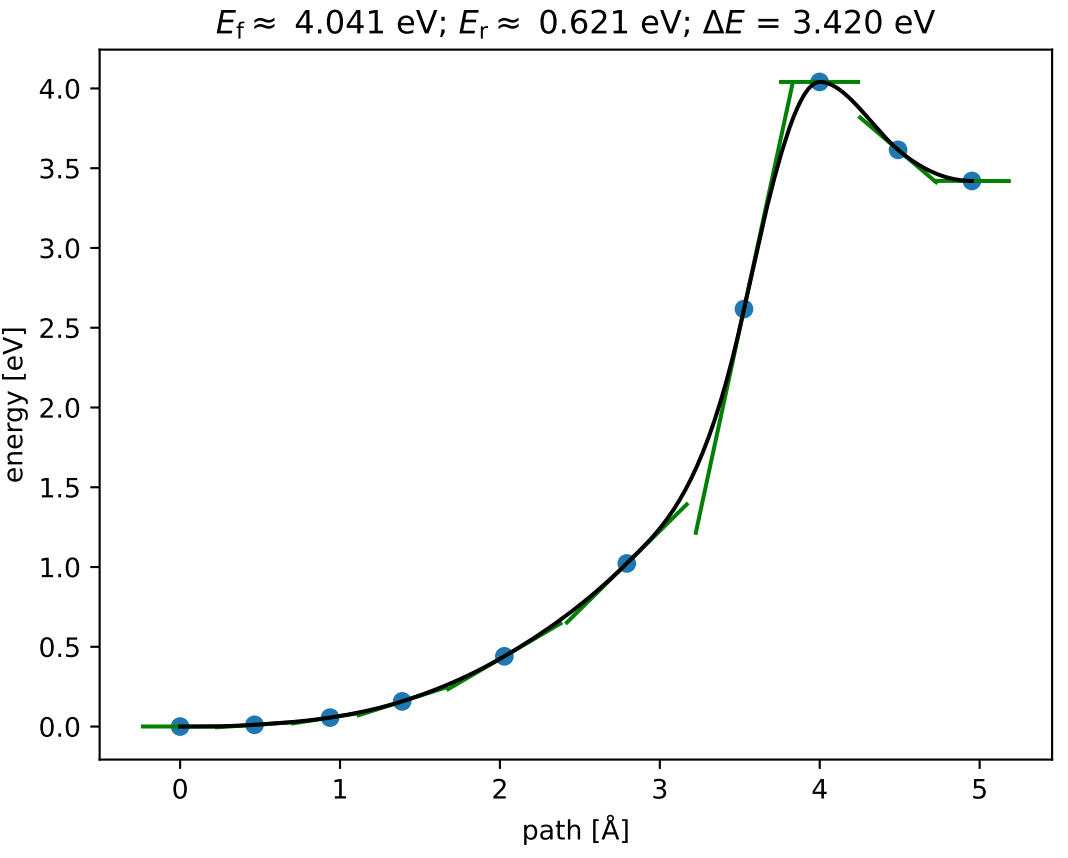
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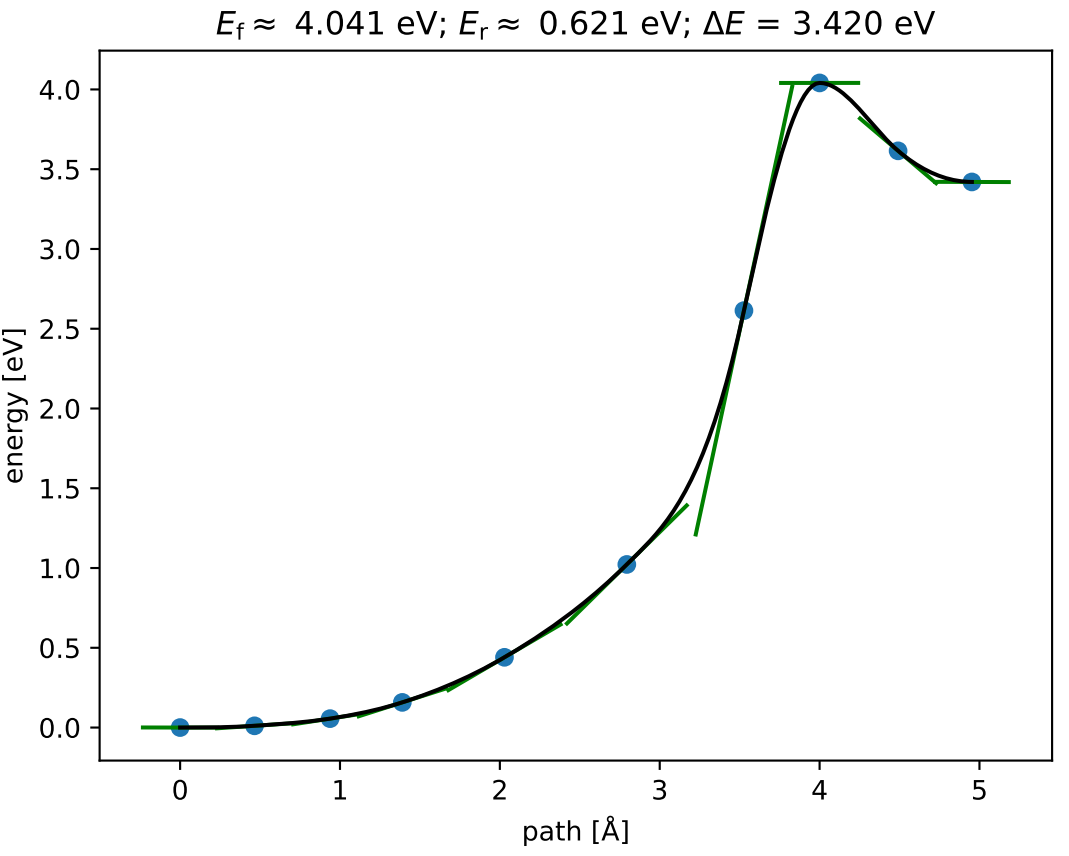
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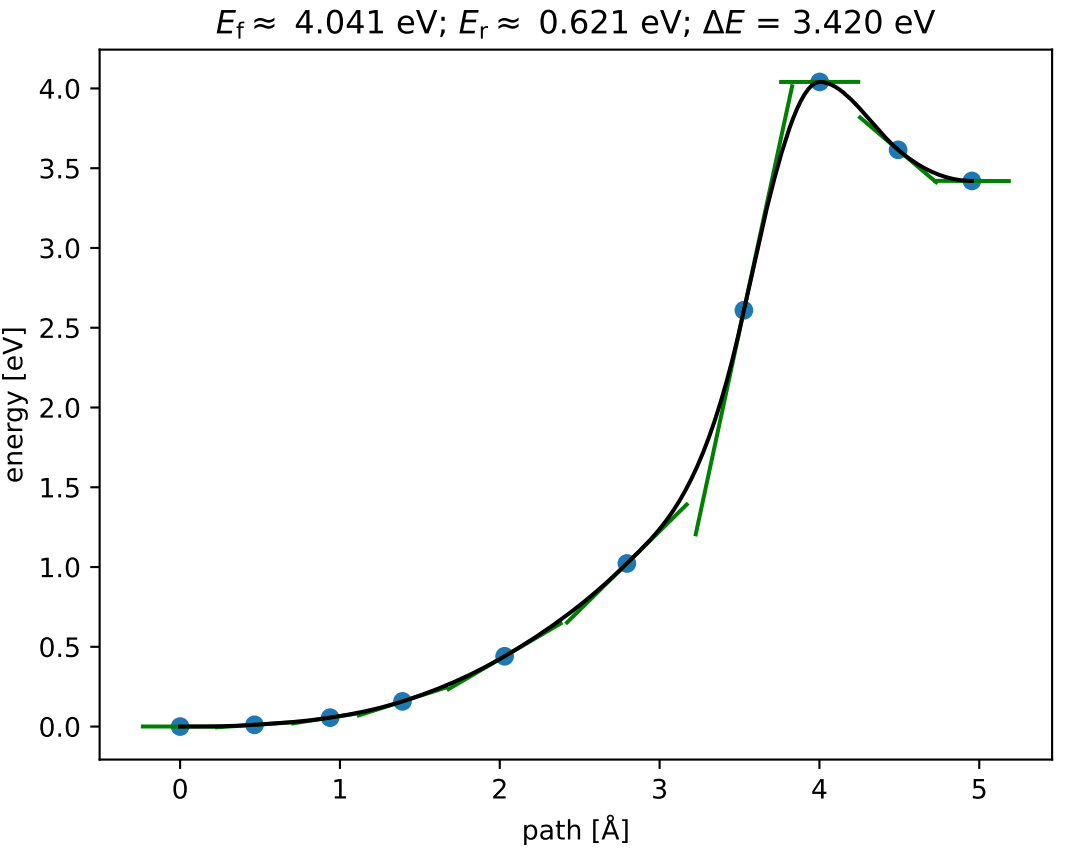
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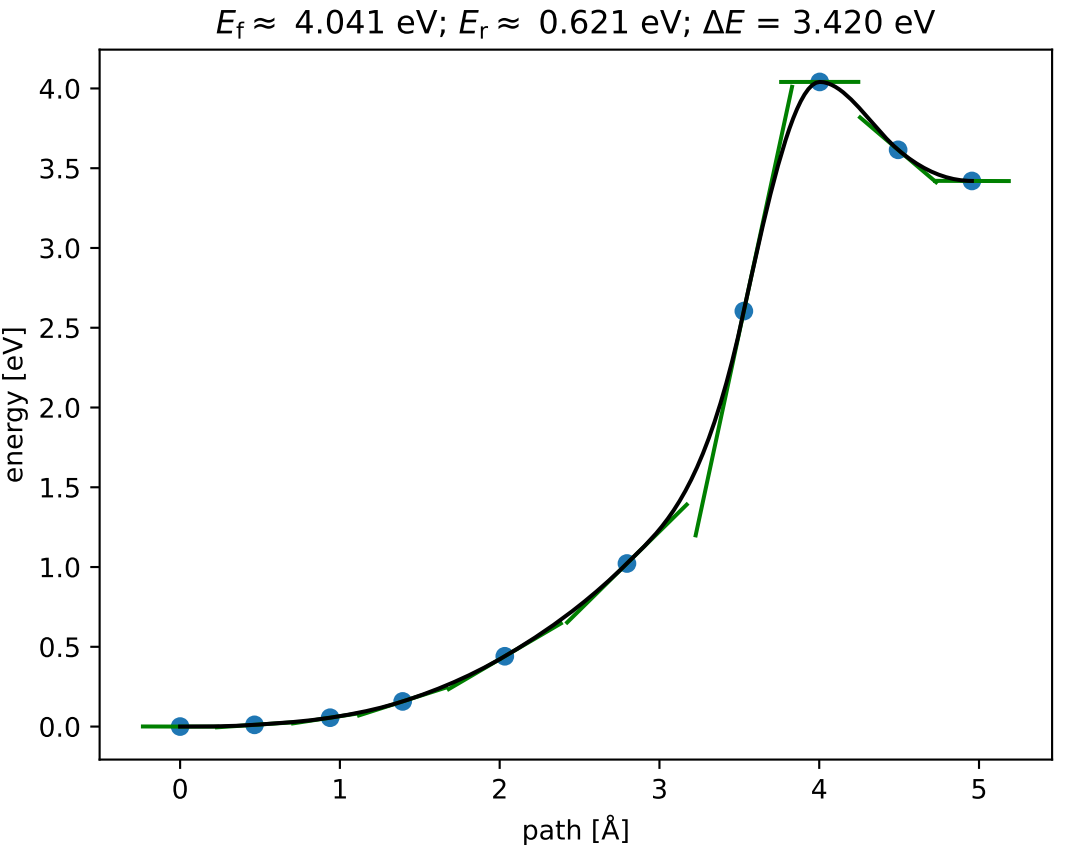
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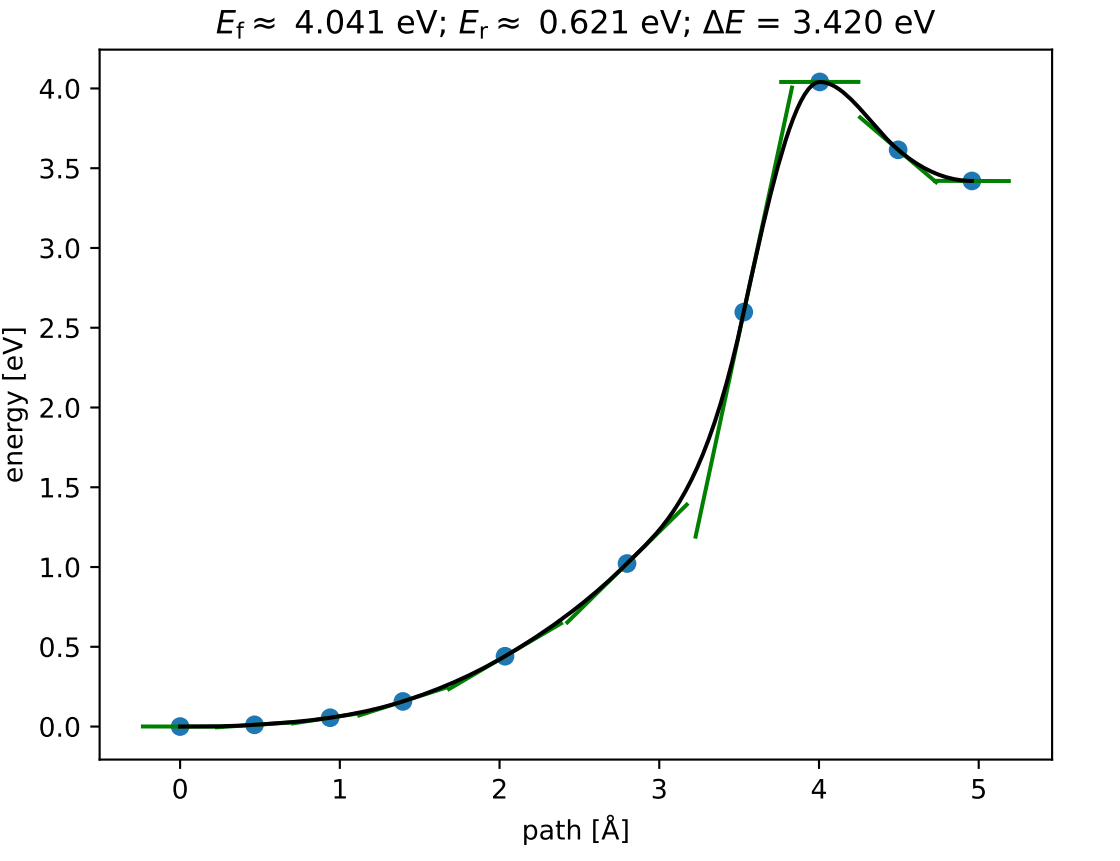
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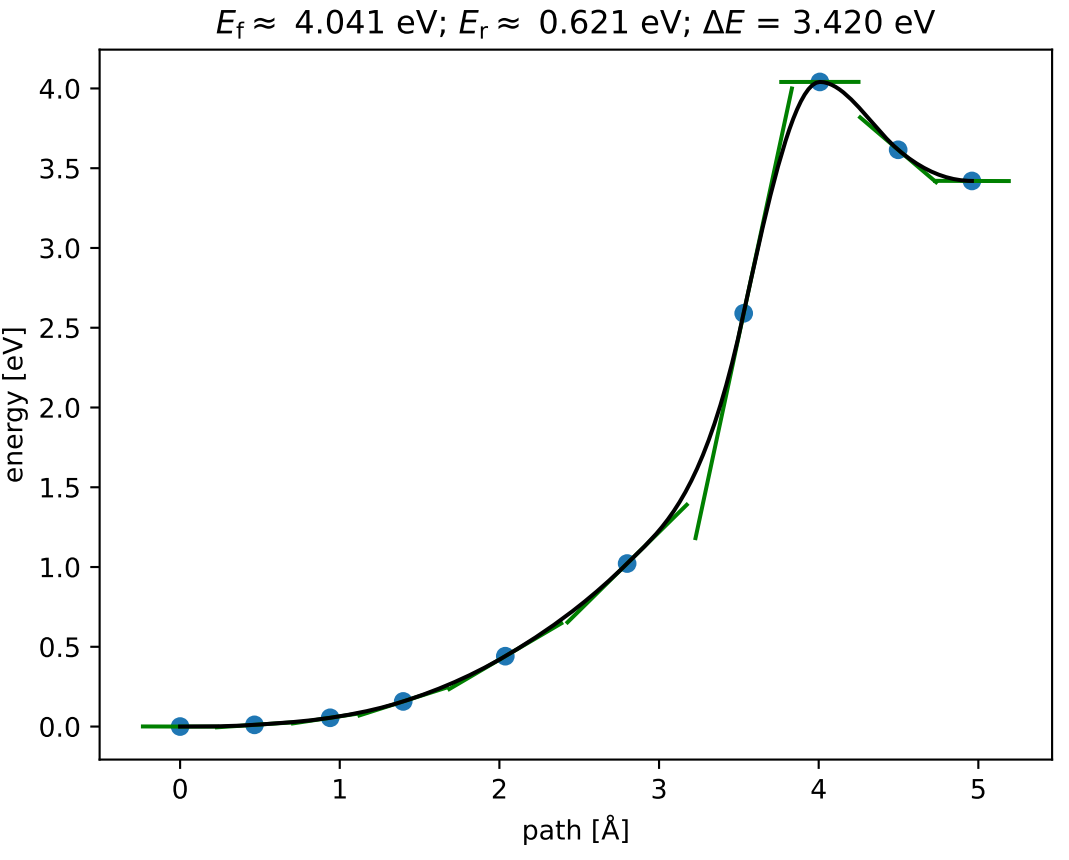
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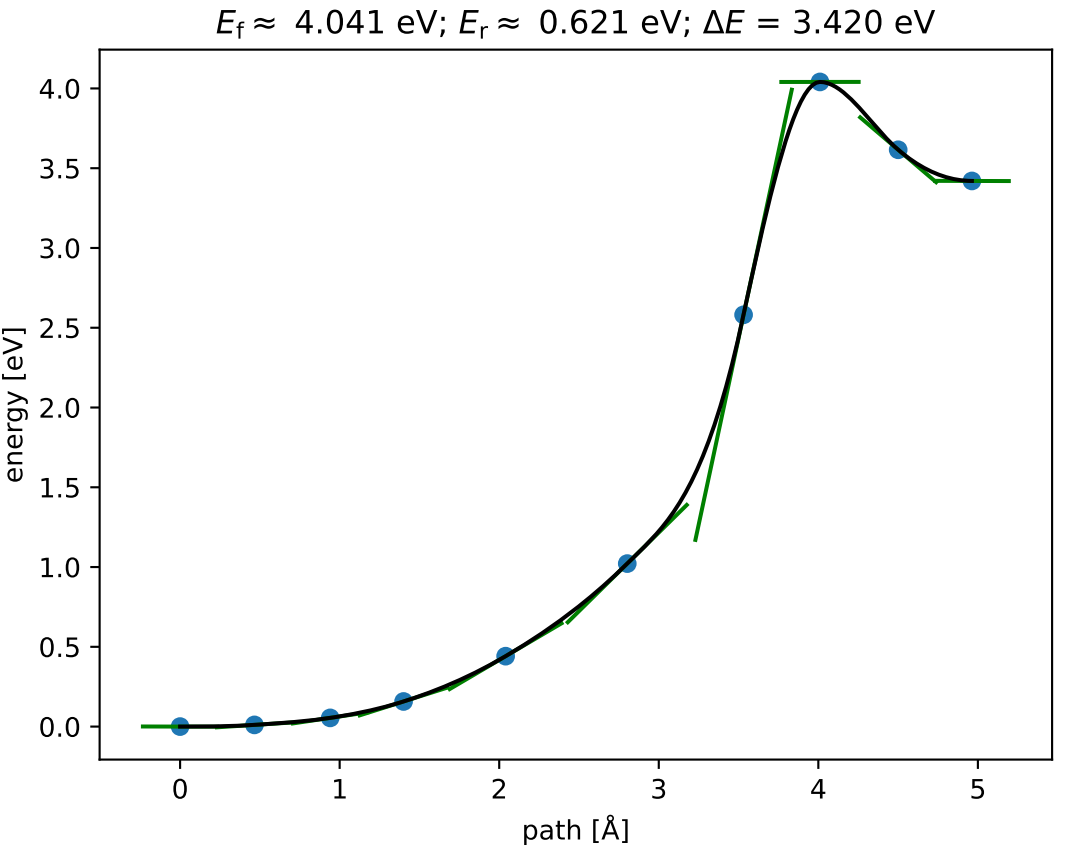
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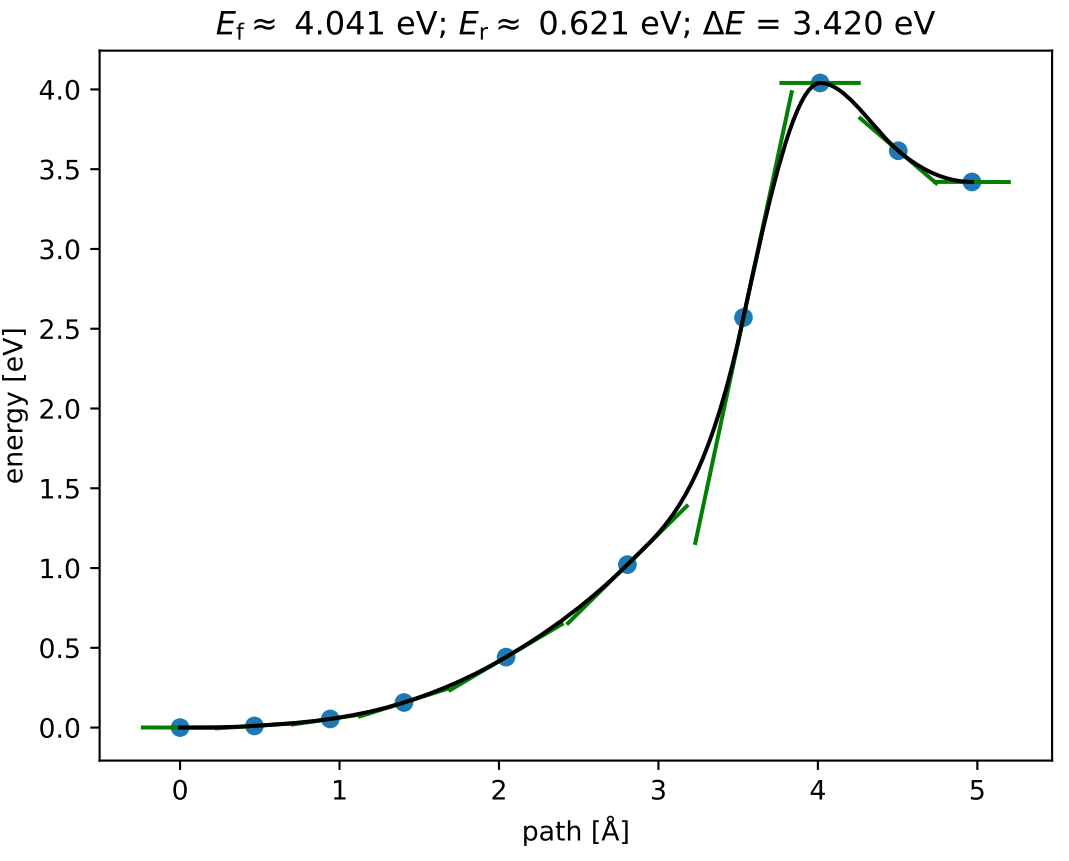
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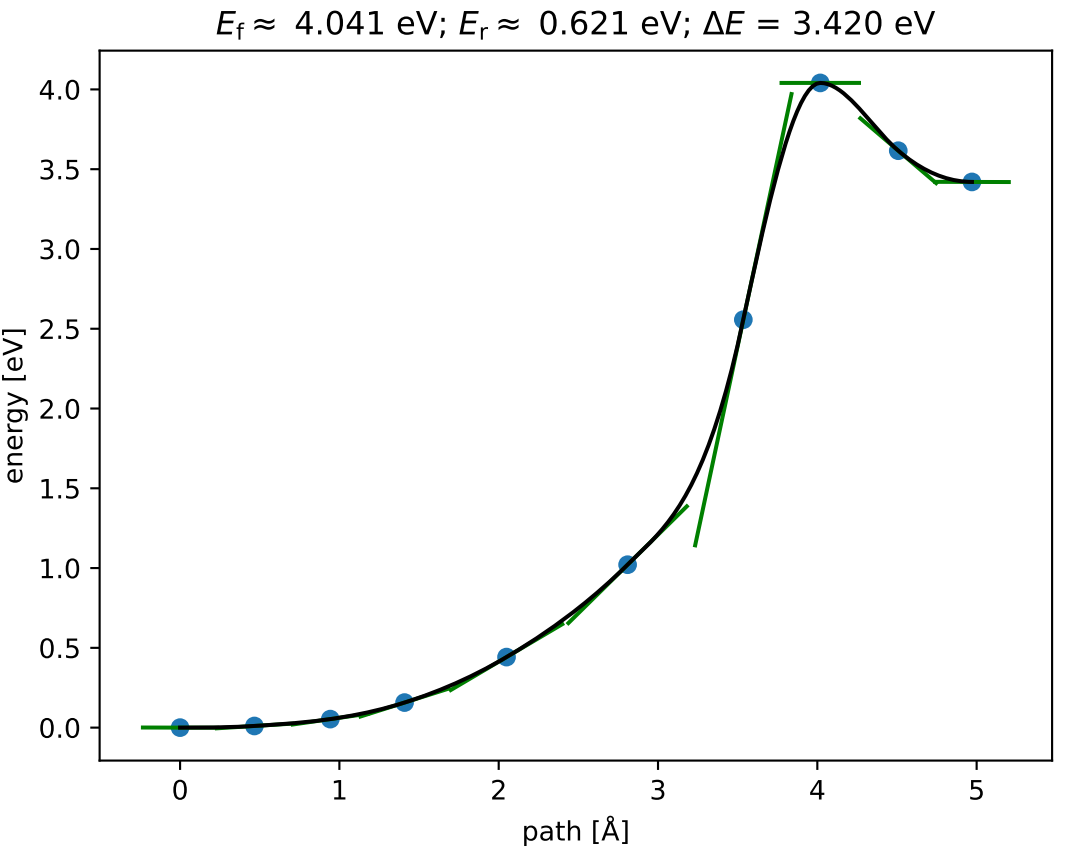
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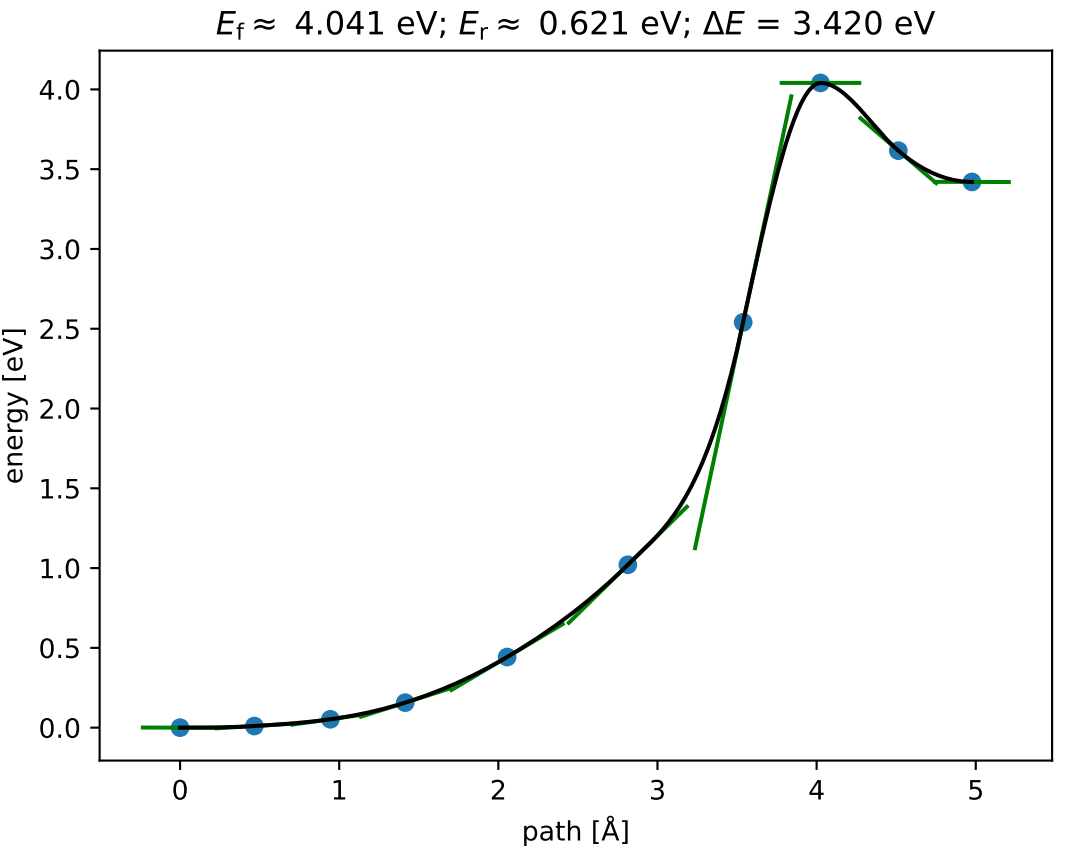
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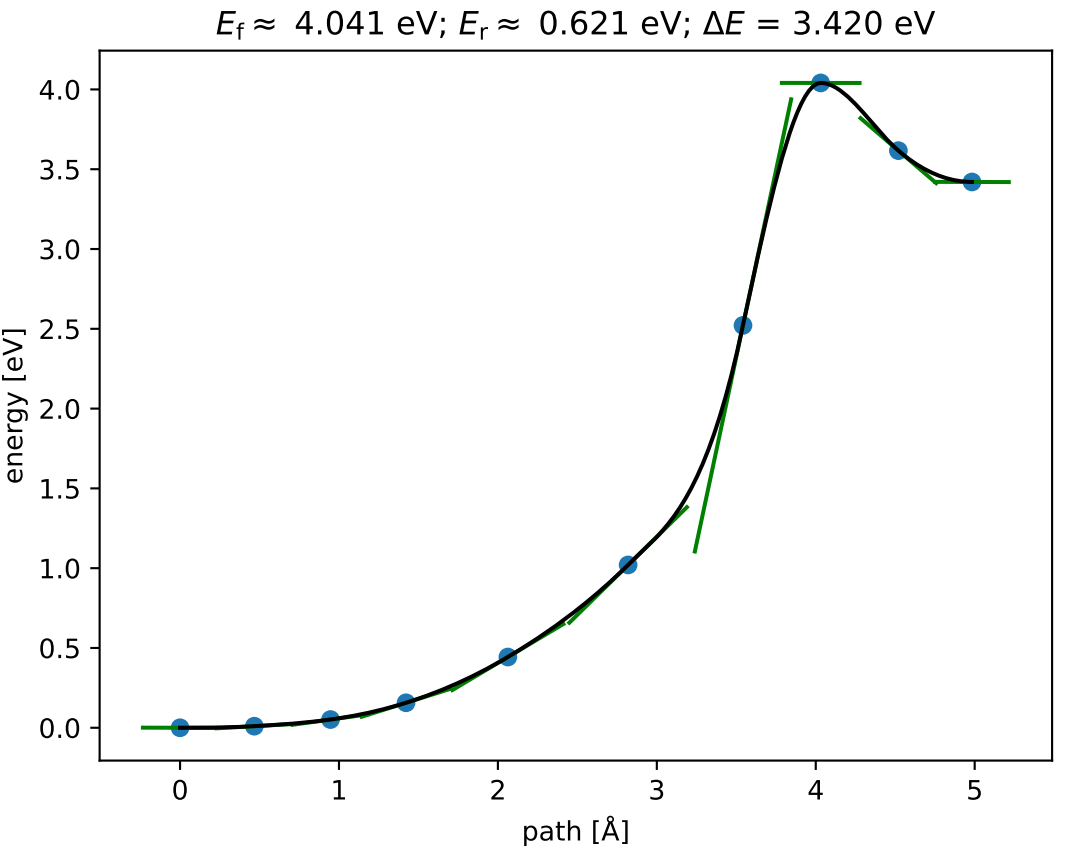
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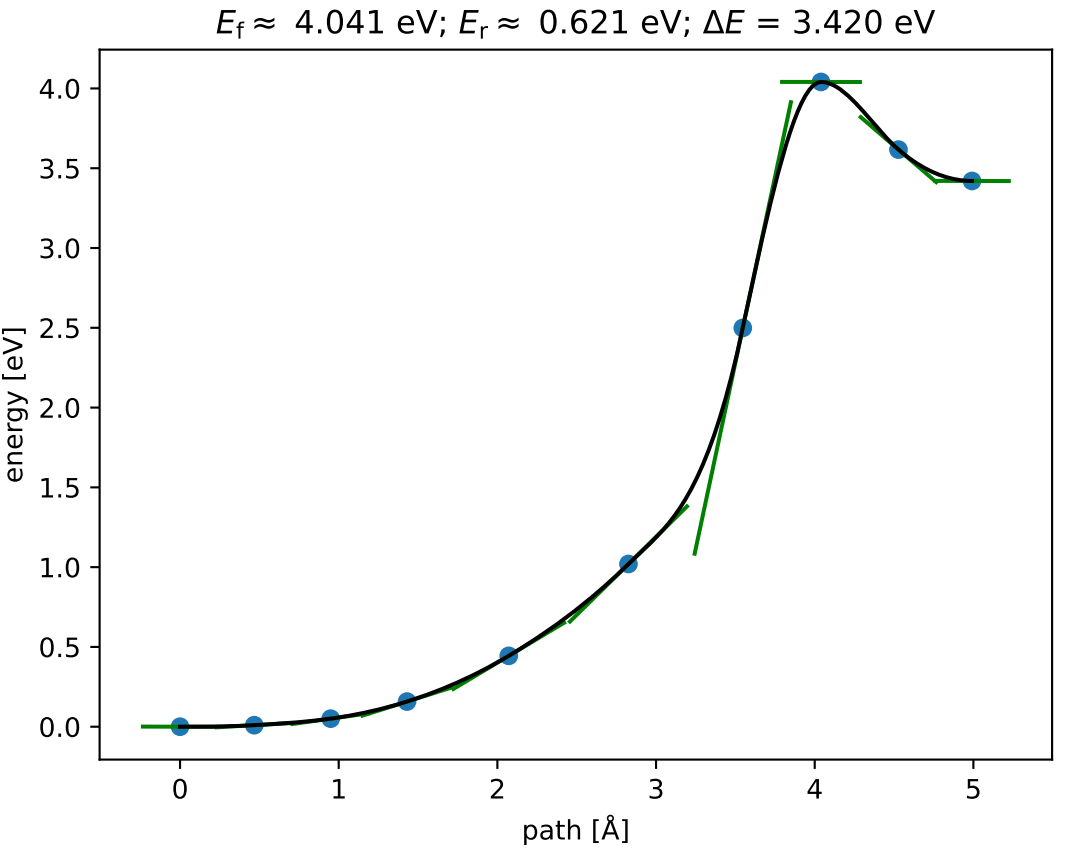
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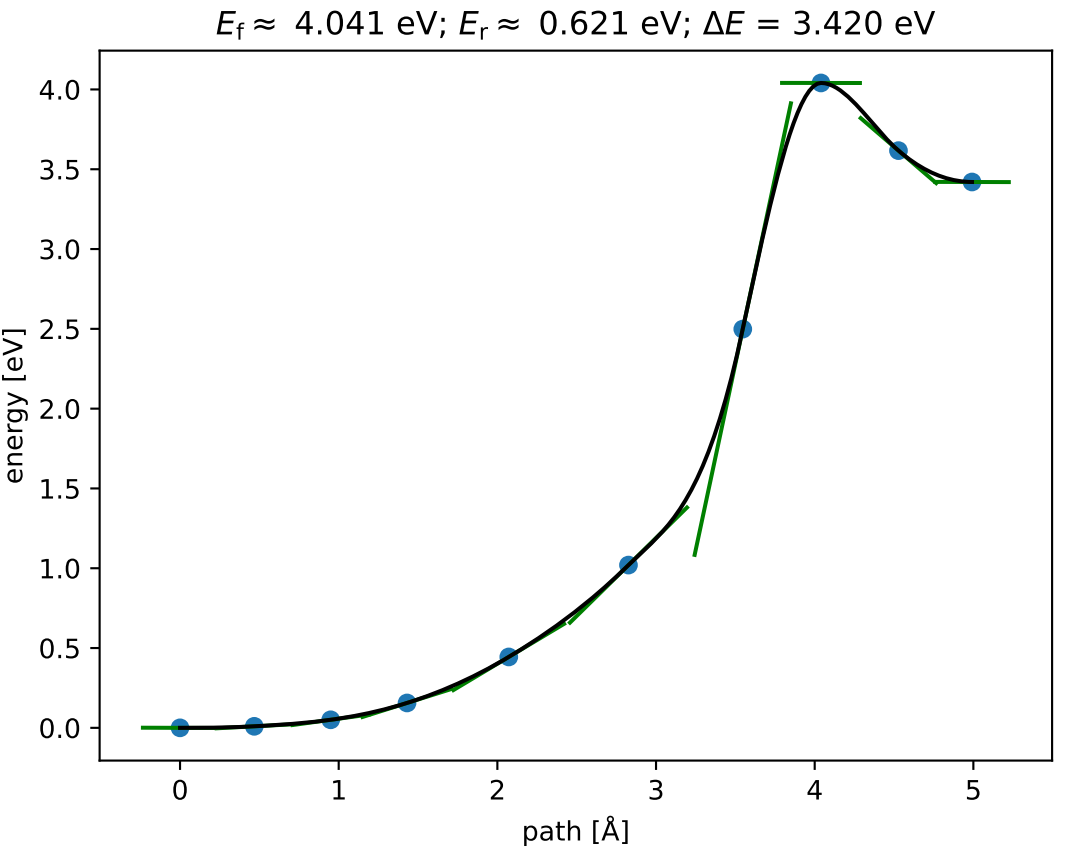
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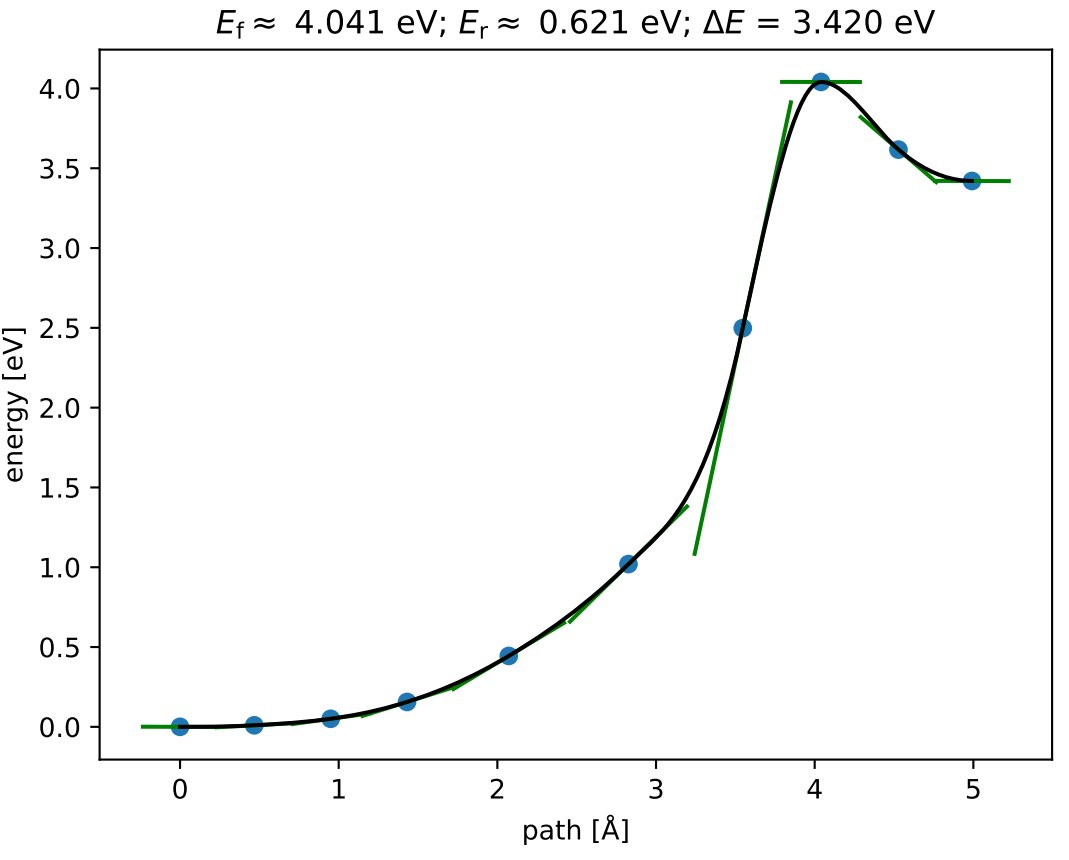
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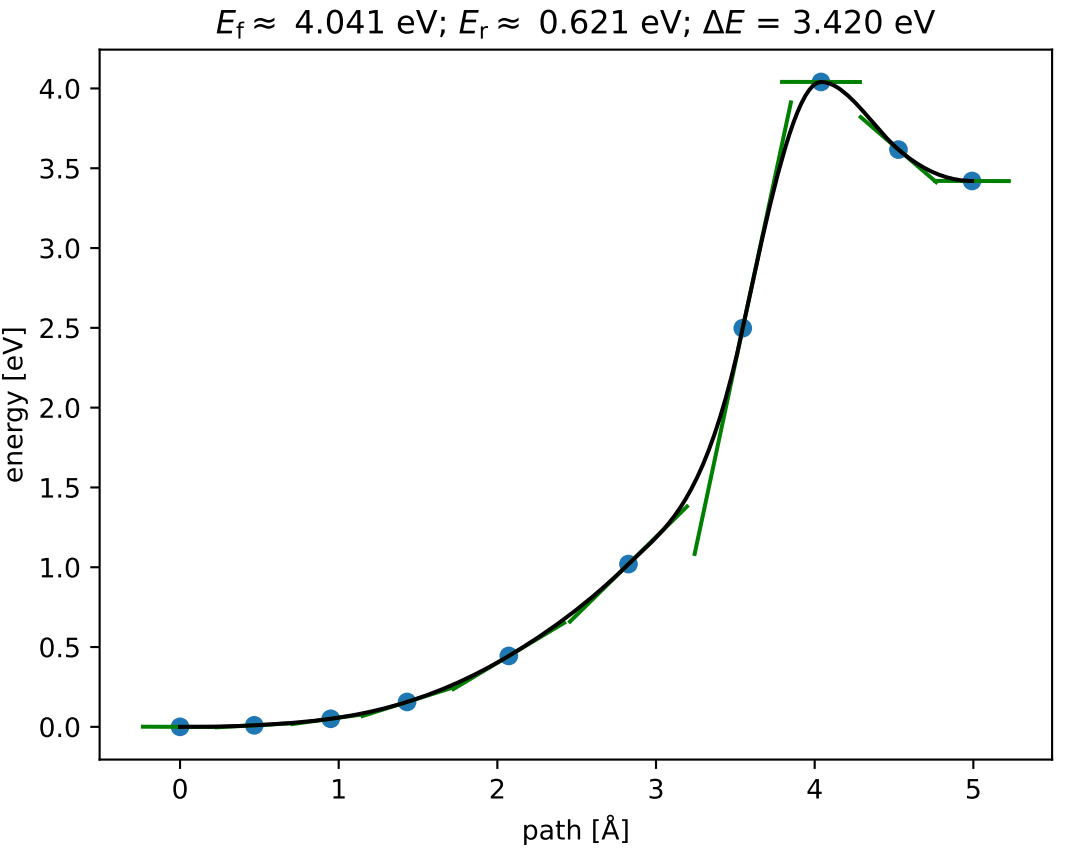
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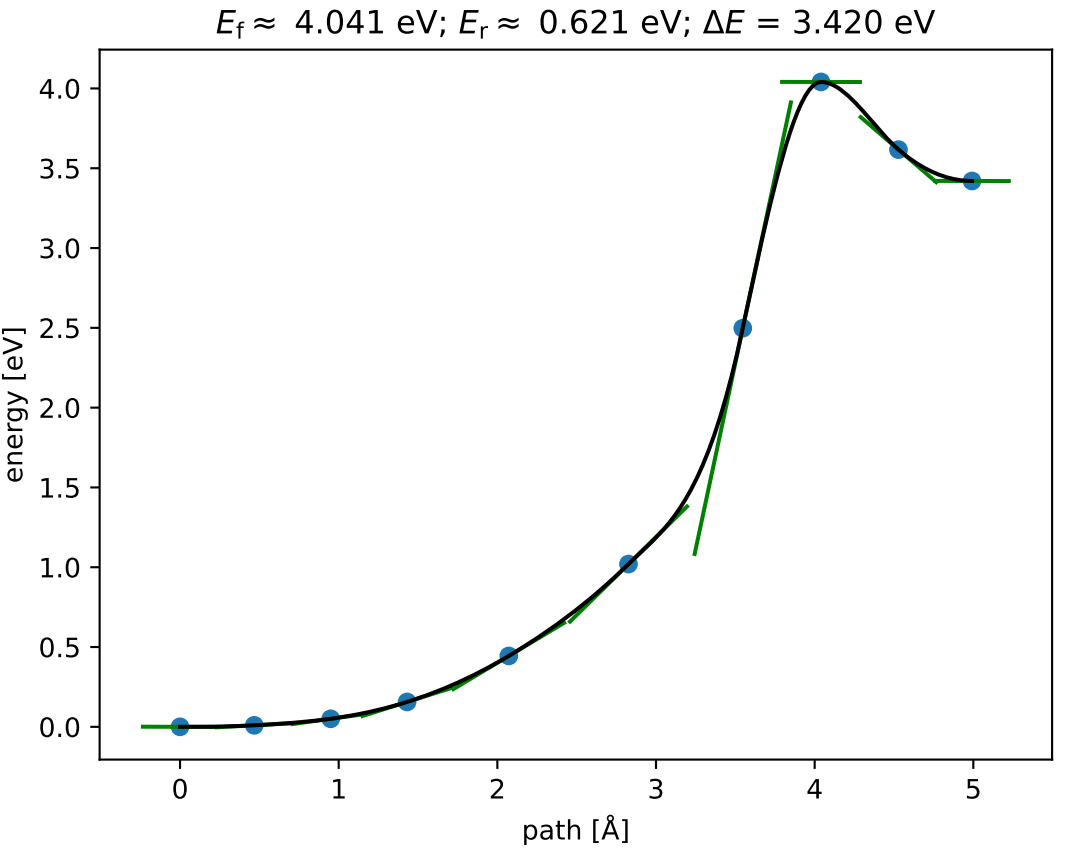
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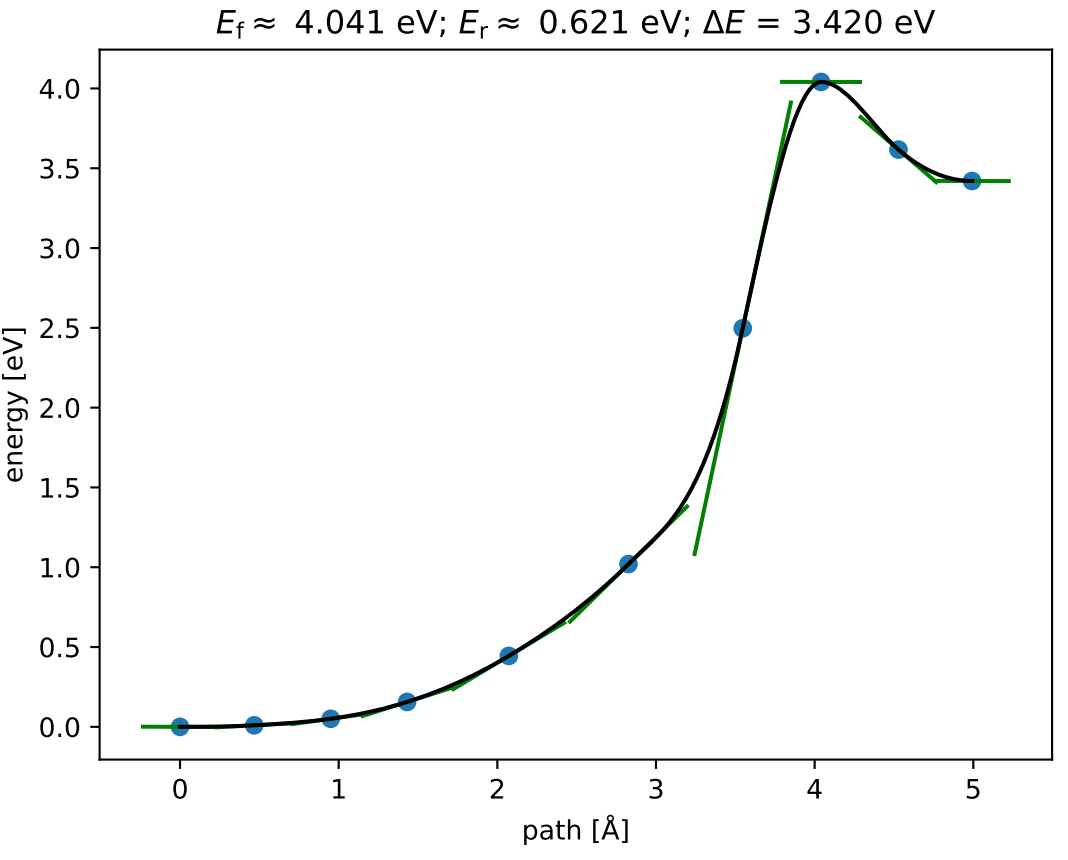
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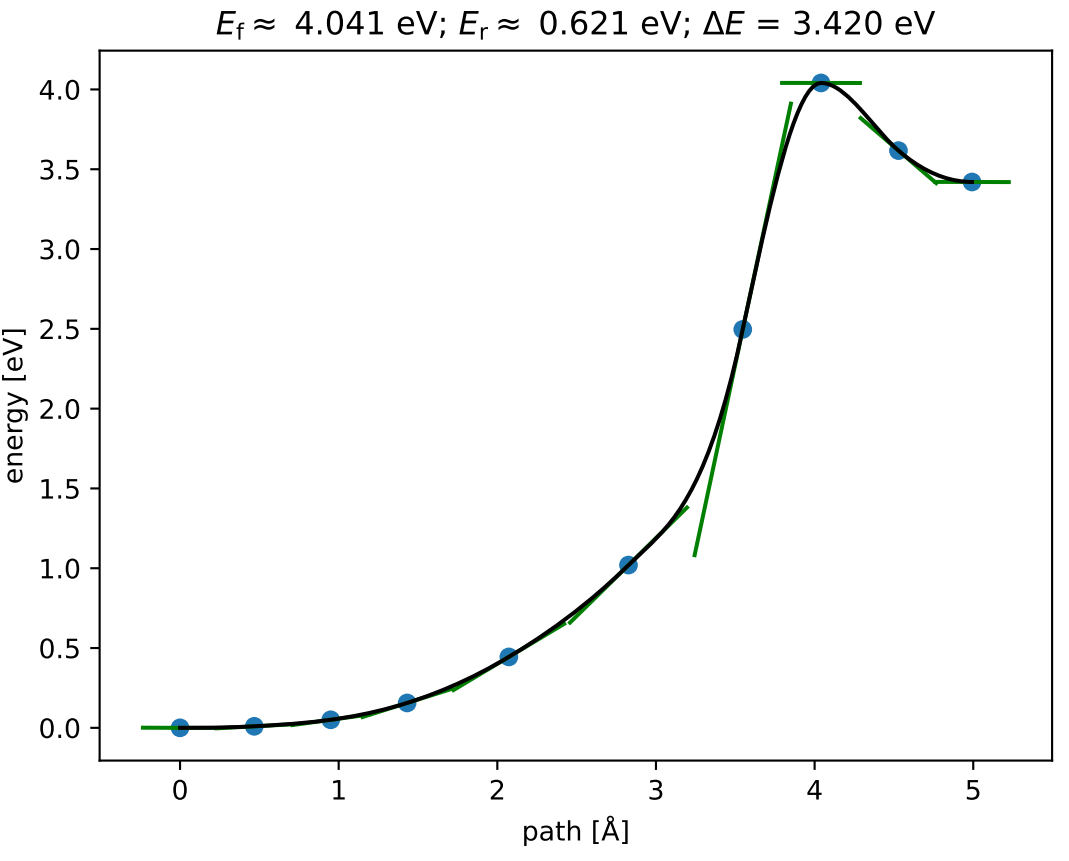
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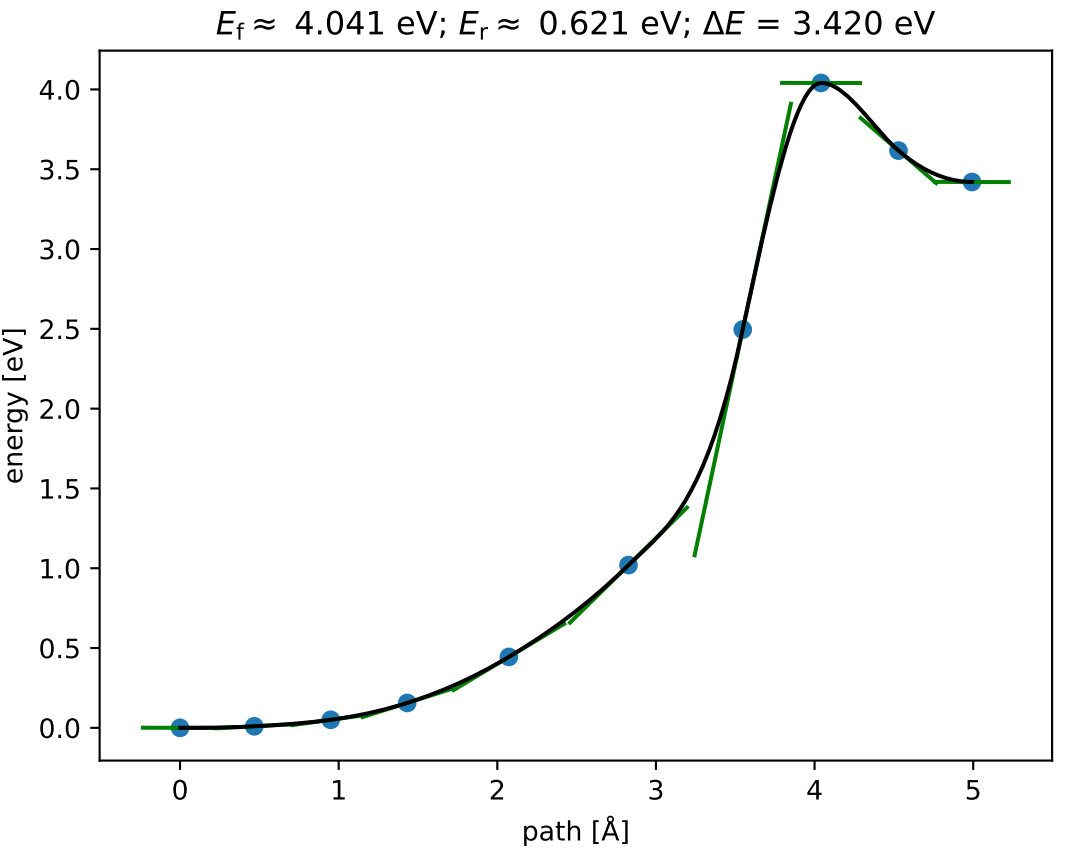
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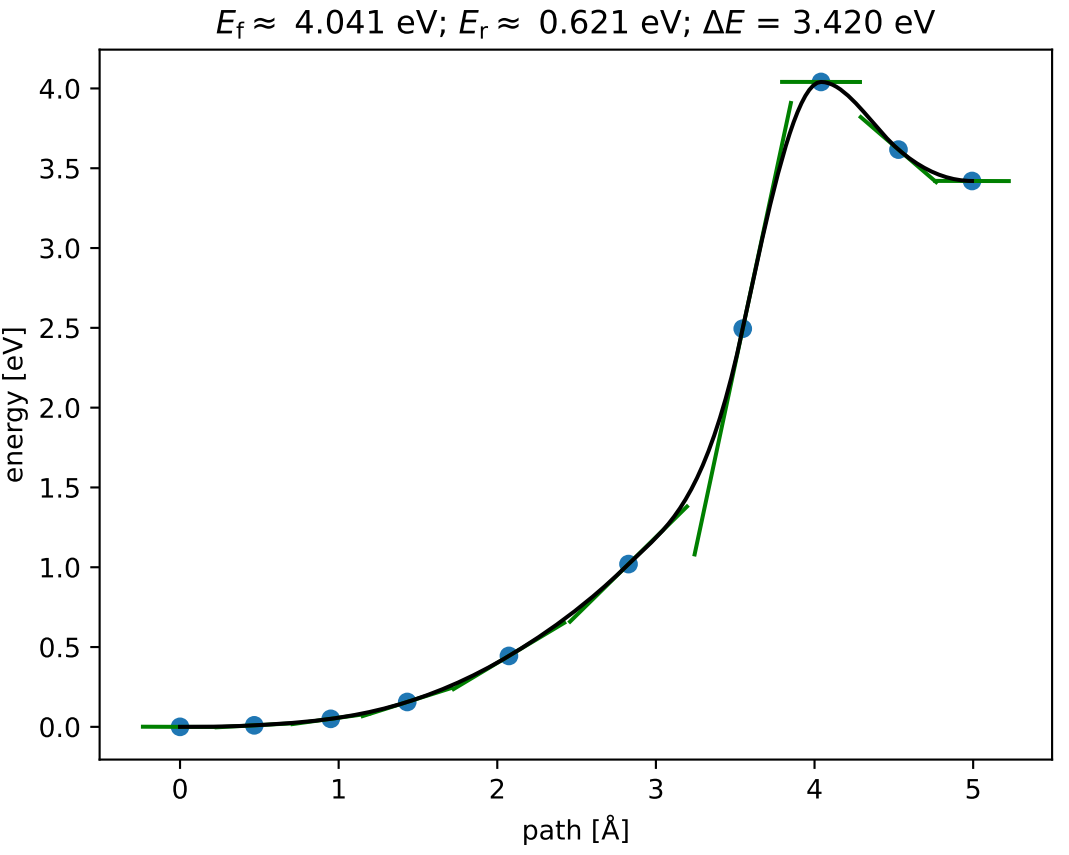
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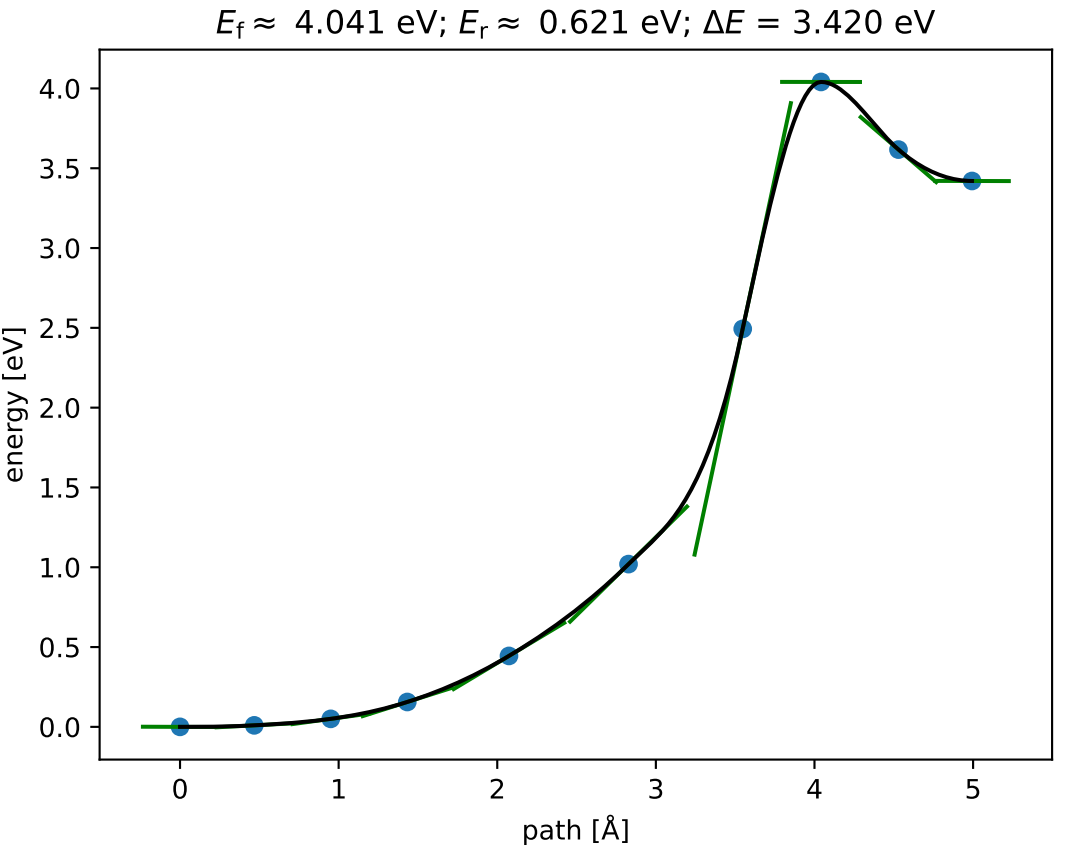
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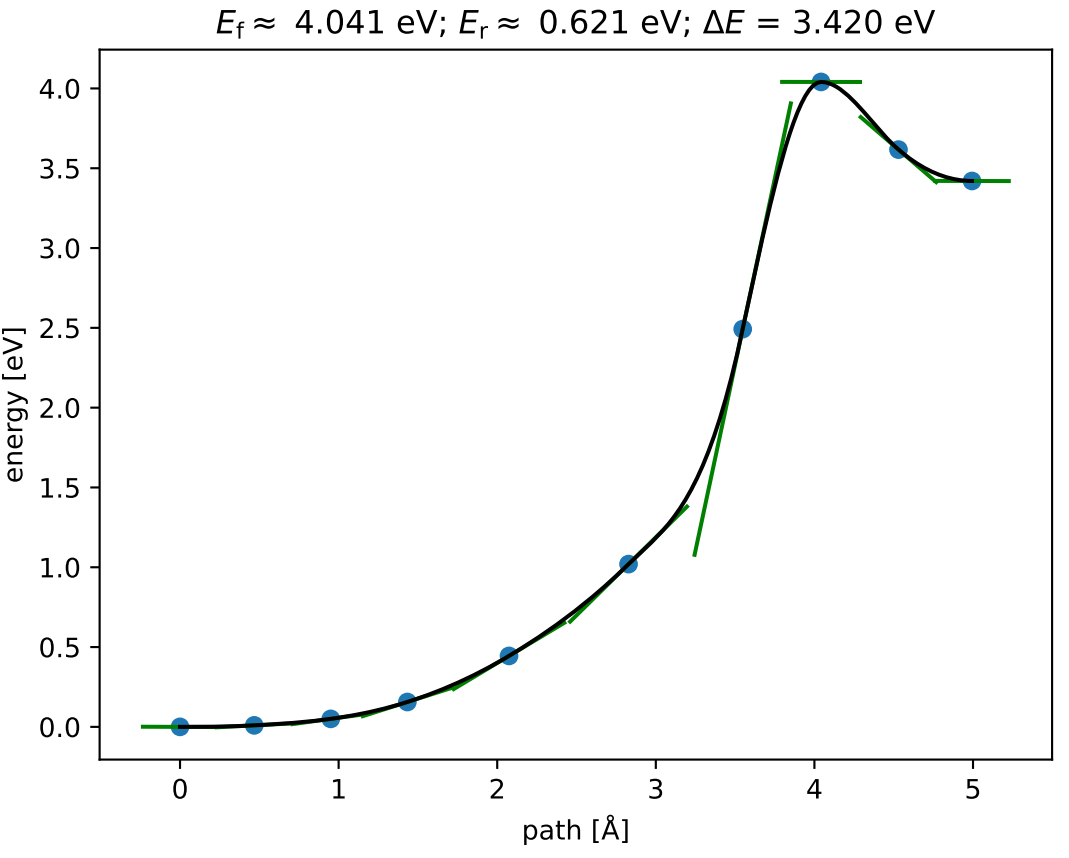
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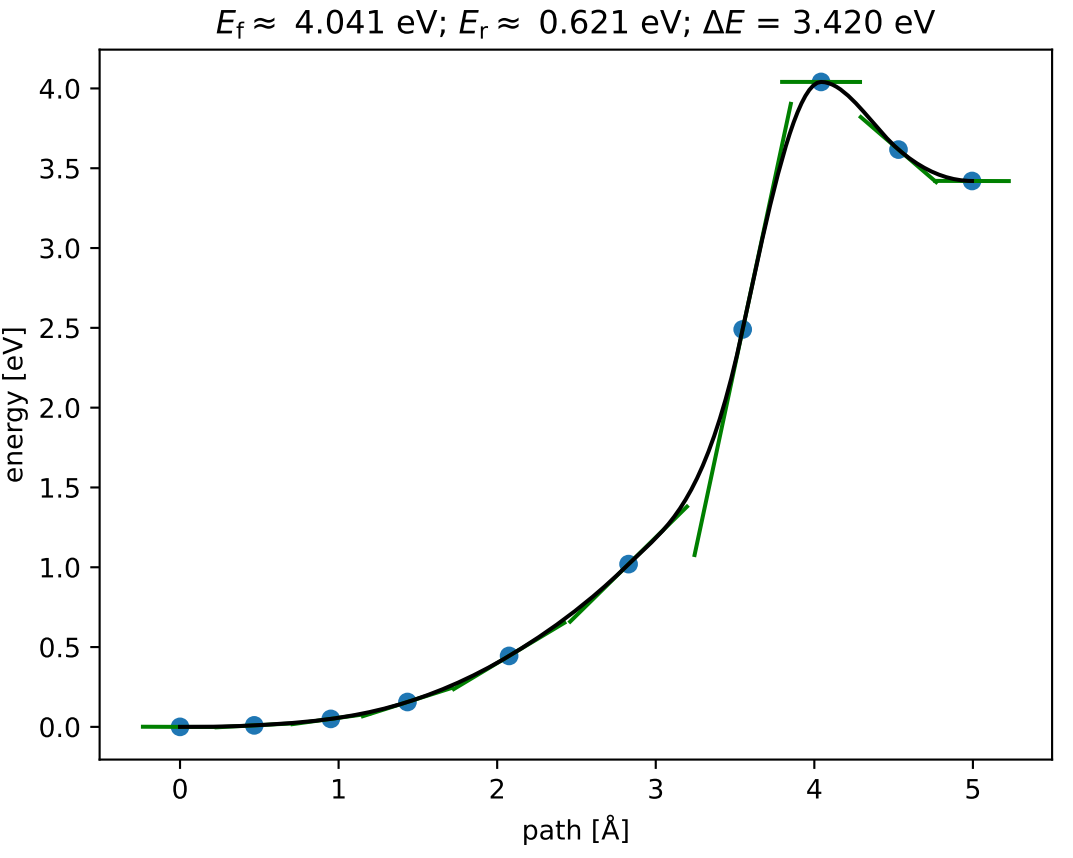
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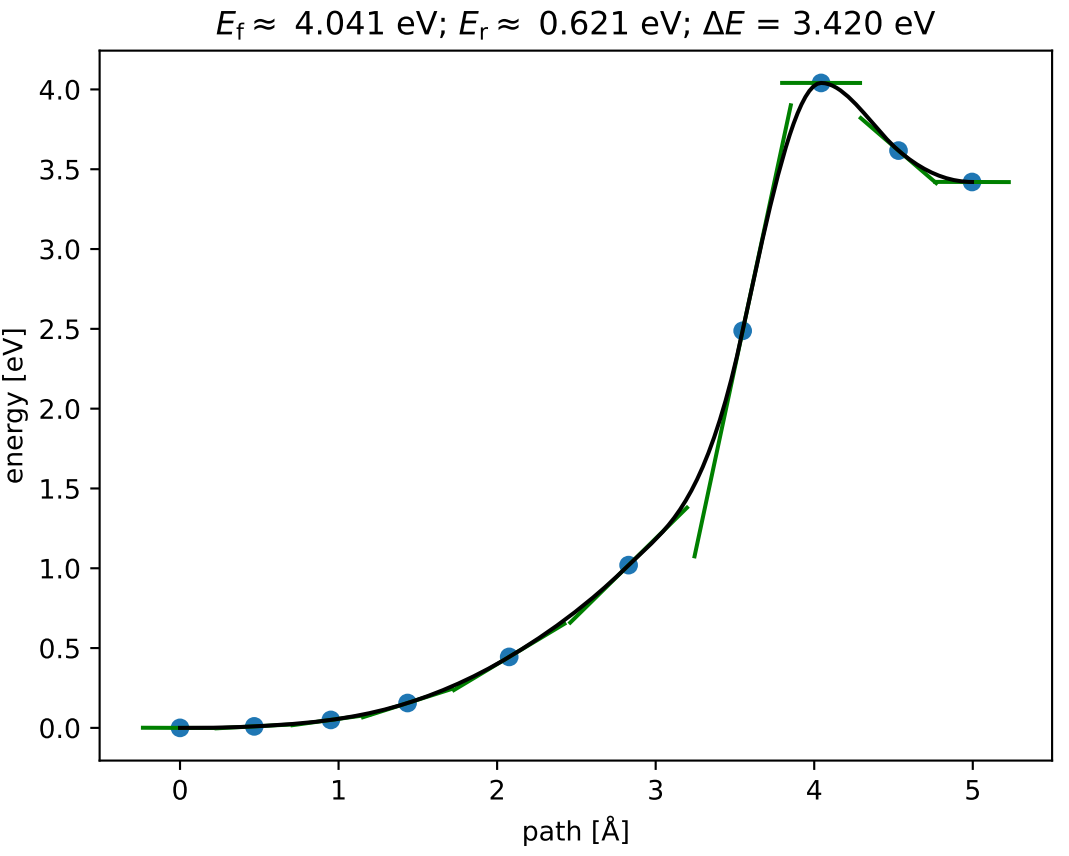
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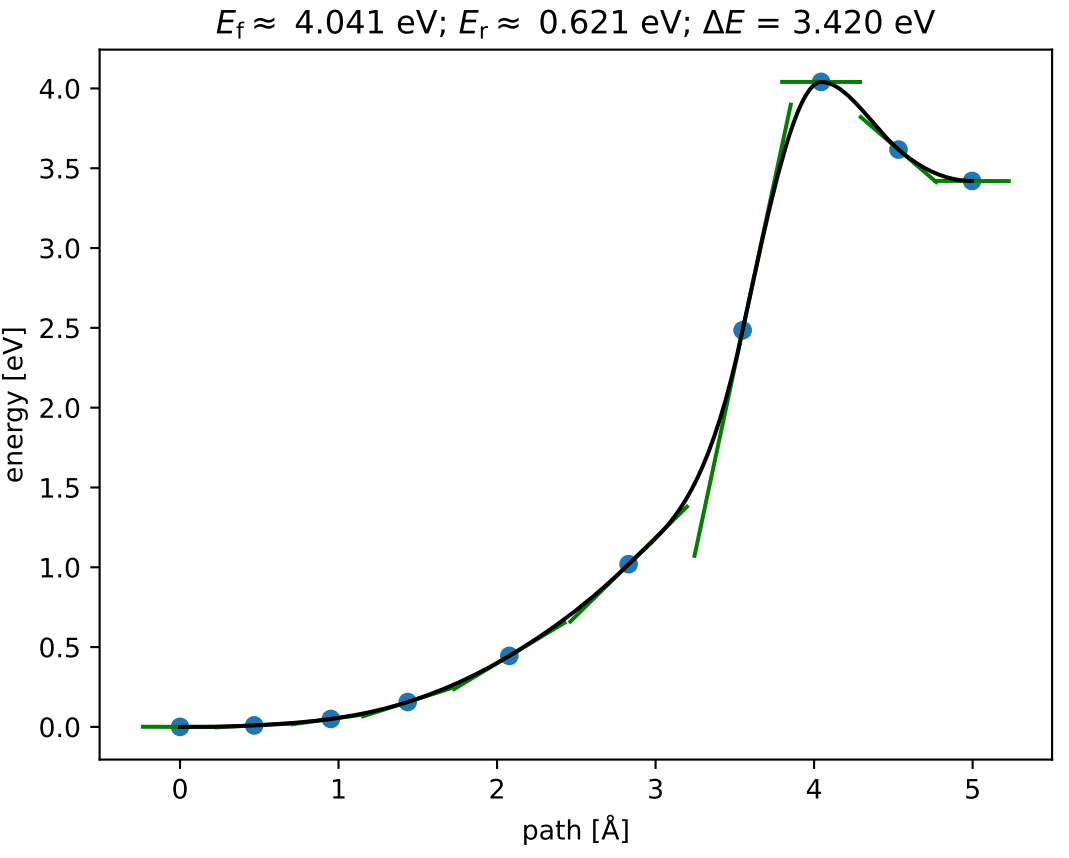
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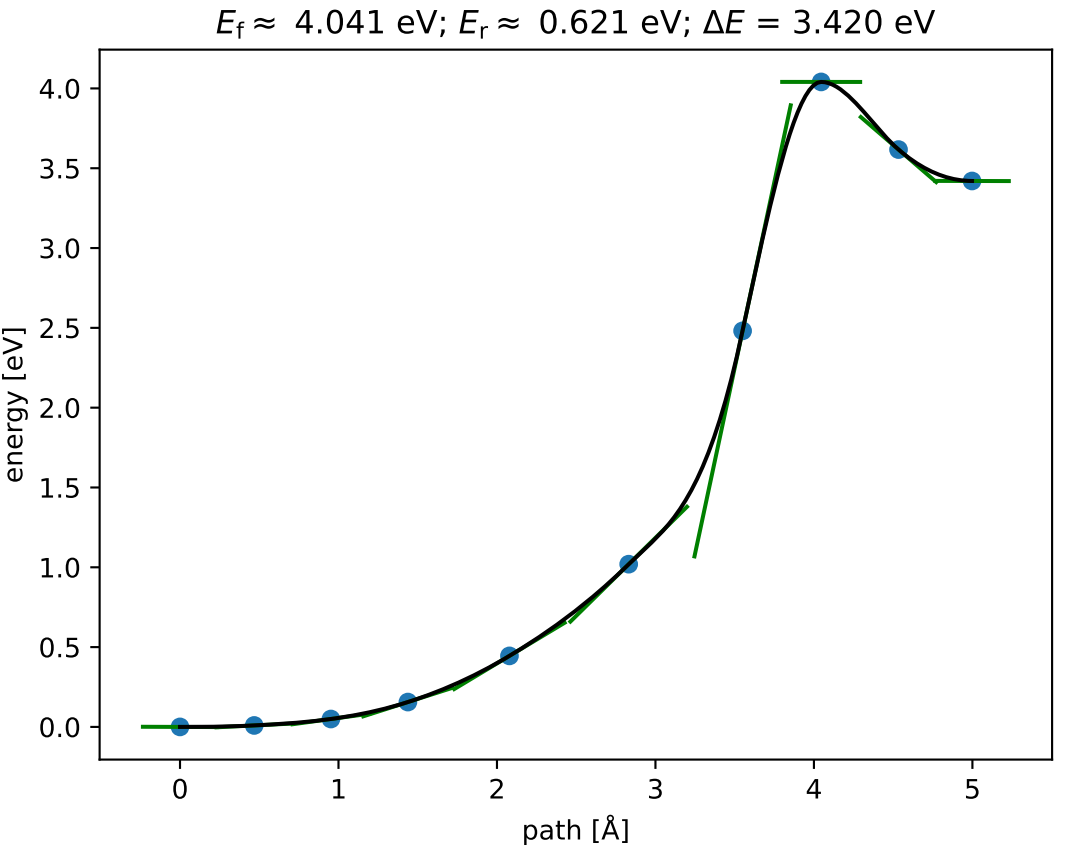
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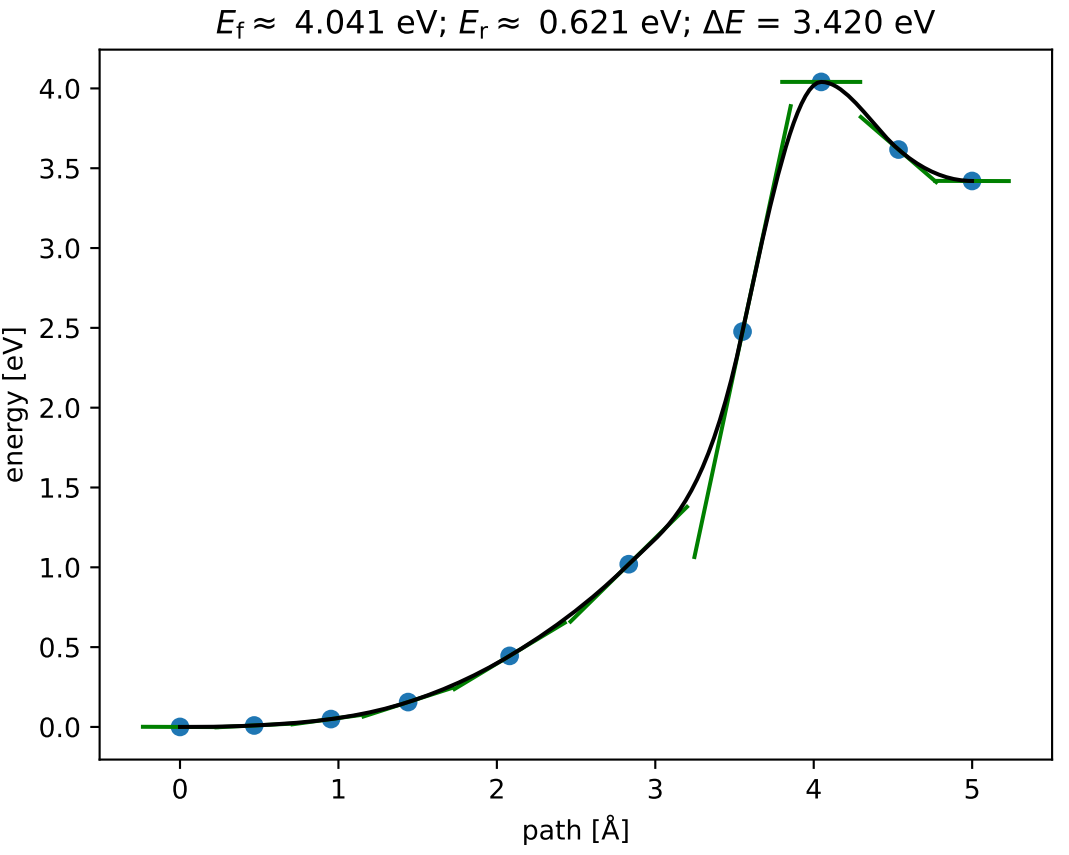
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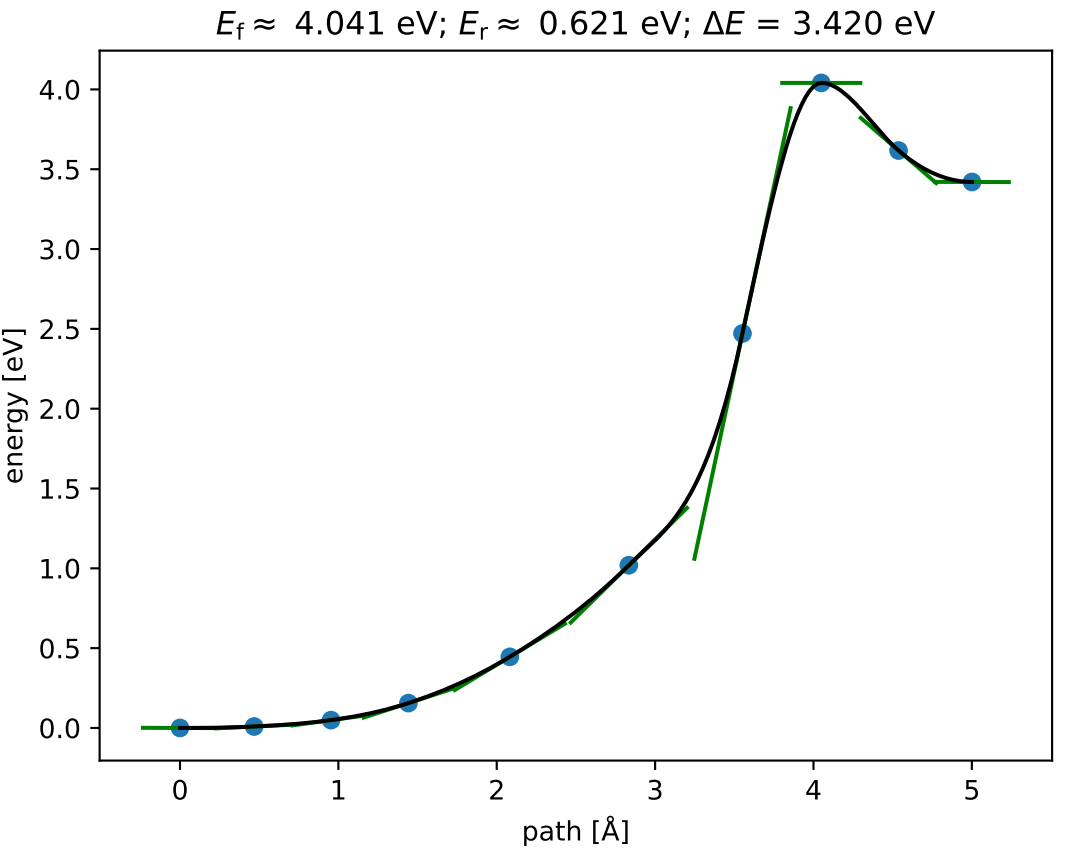
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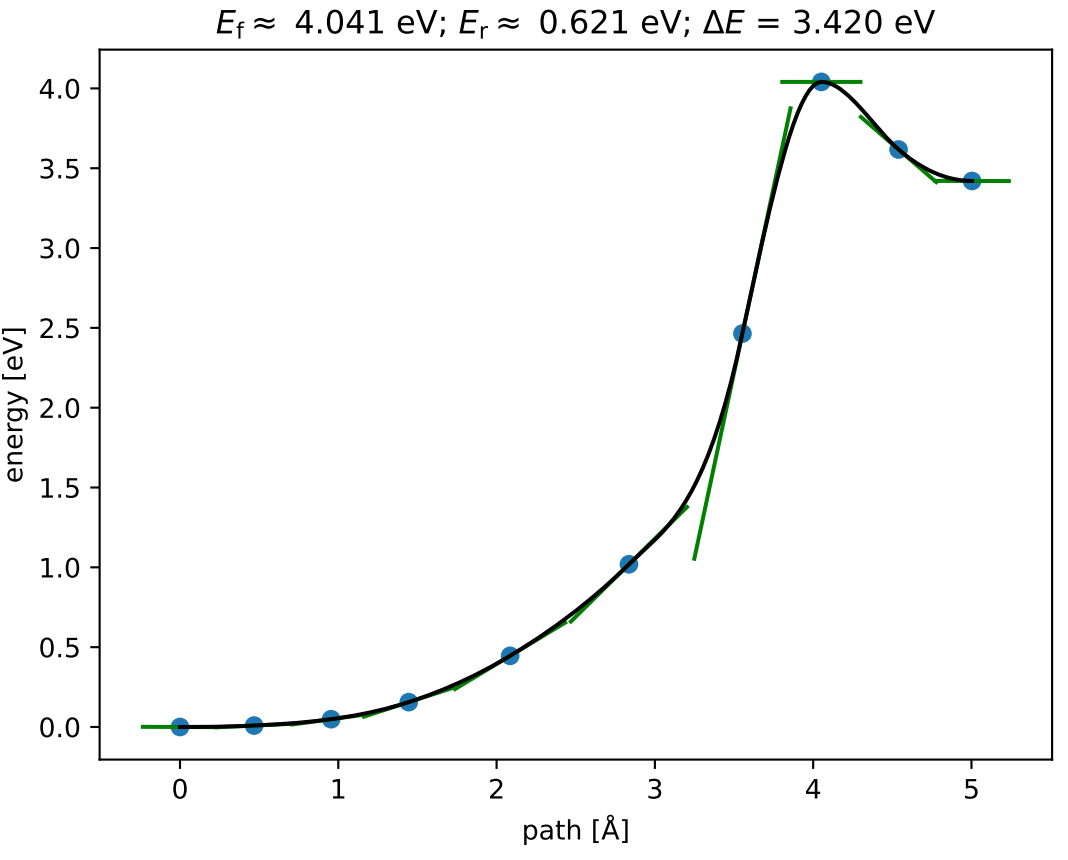
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path [Å]
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1.0
1.5
2.0
2.5
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4.0
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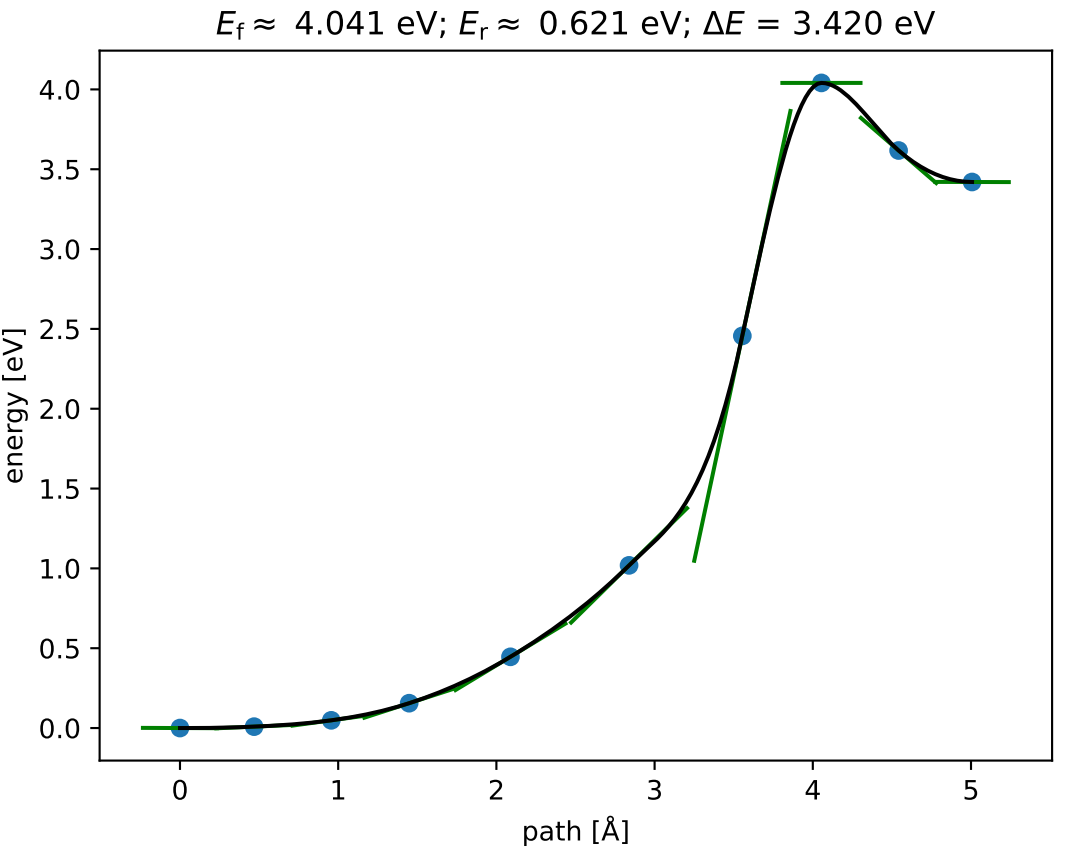
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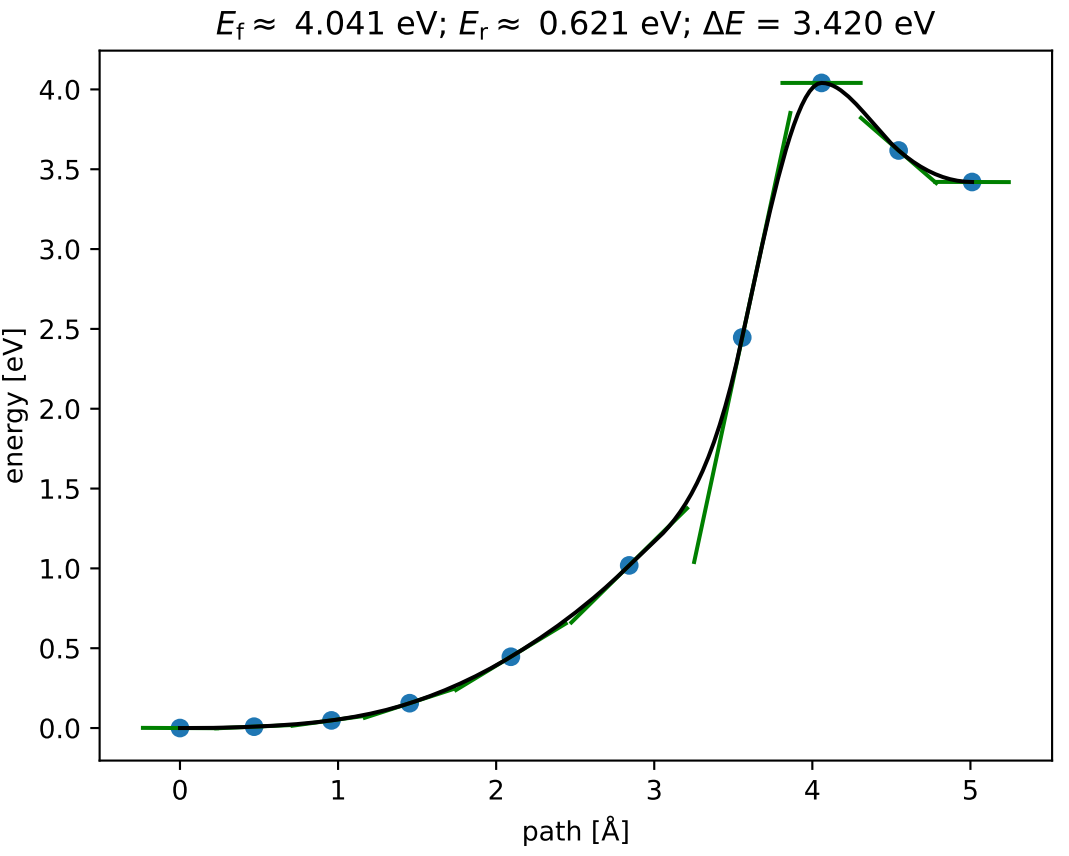
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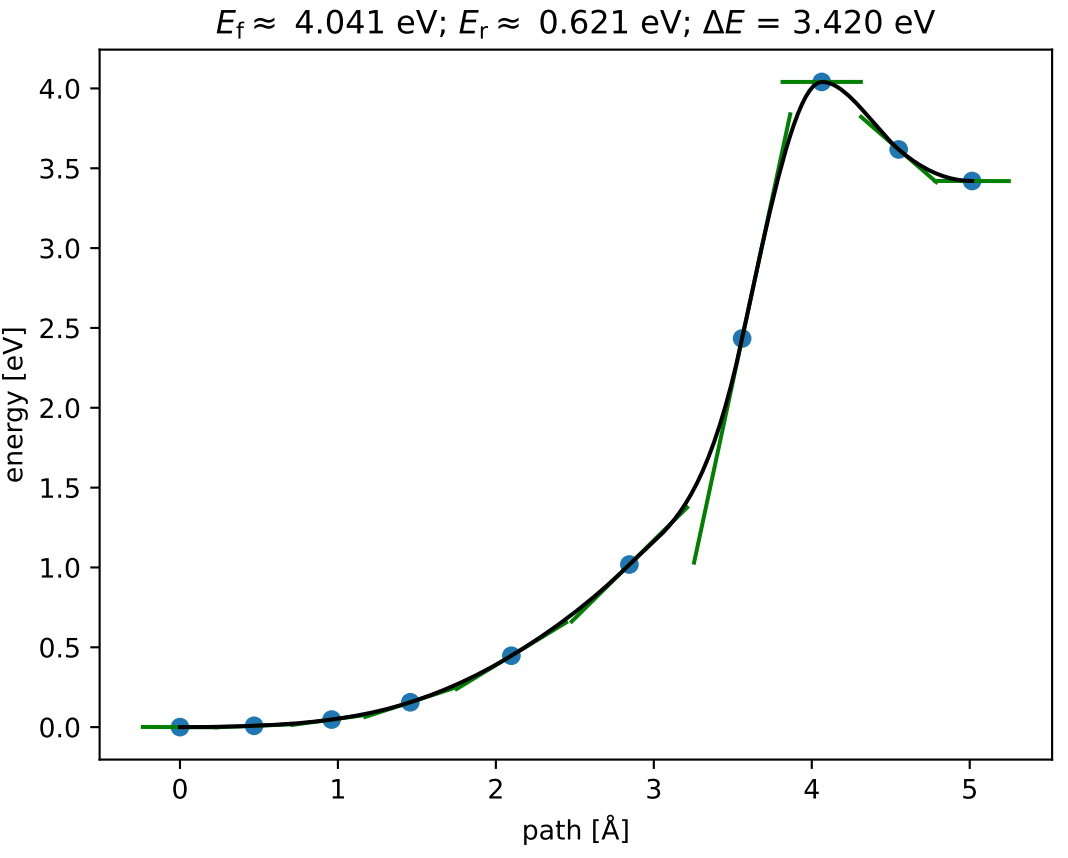
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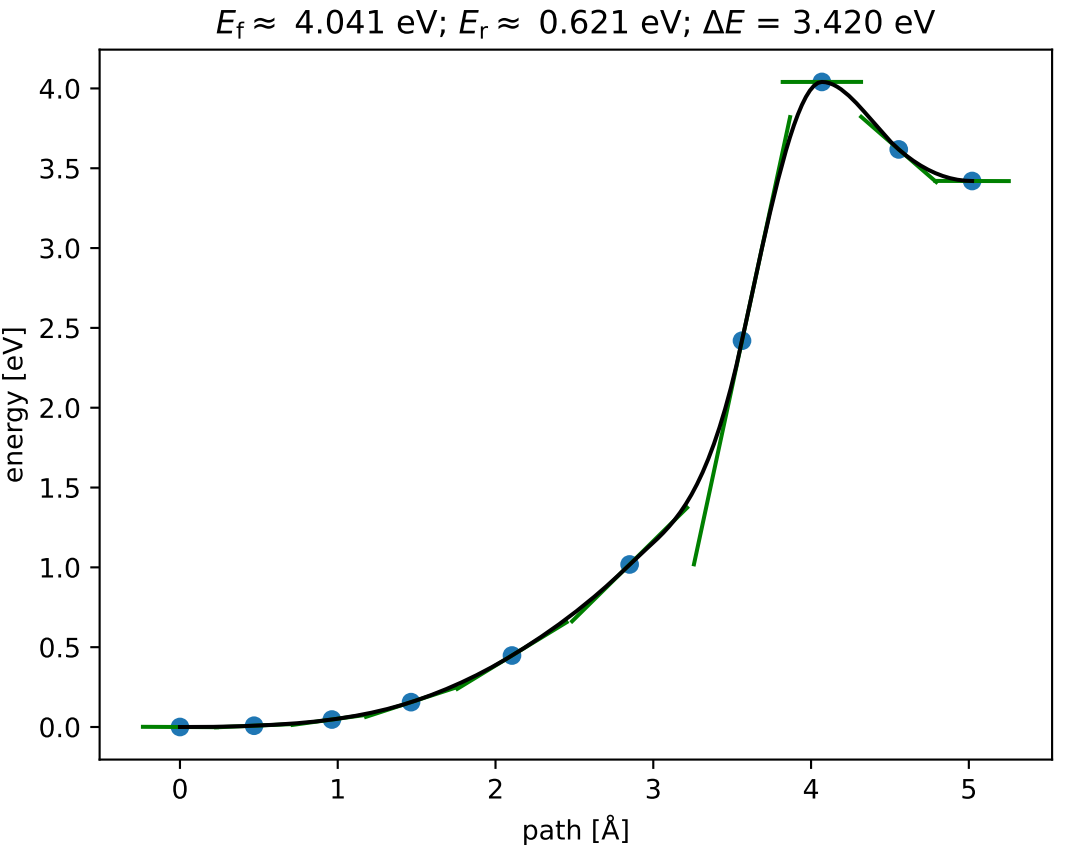
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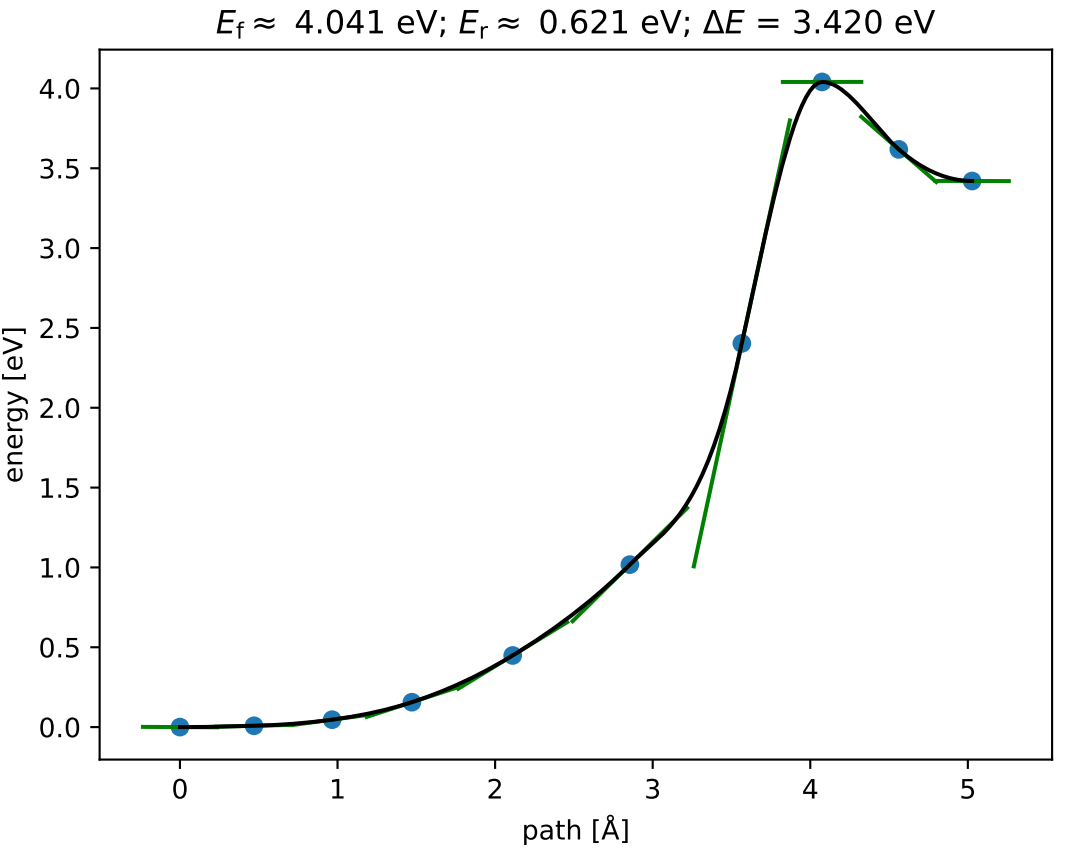
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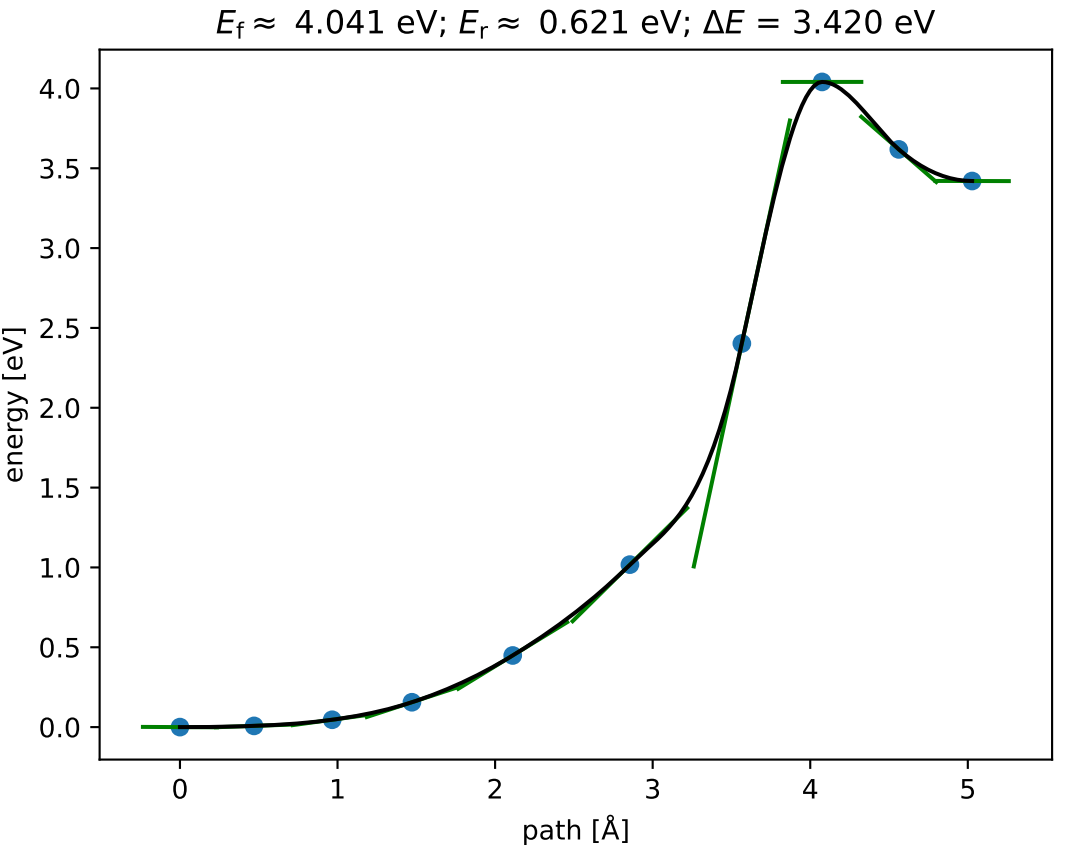
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