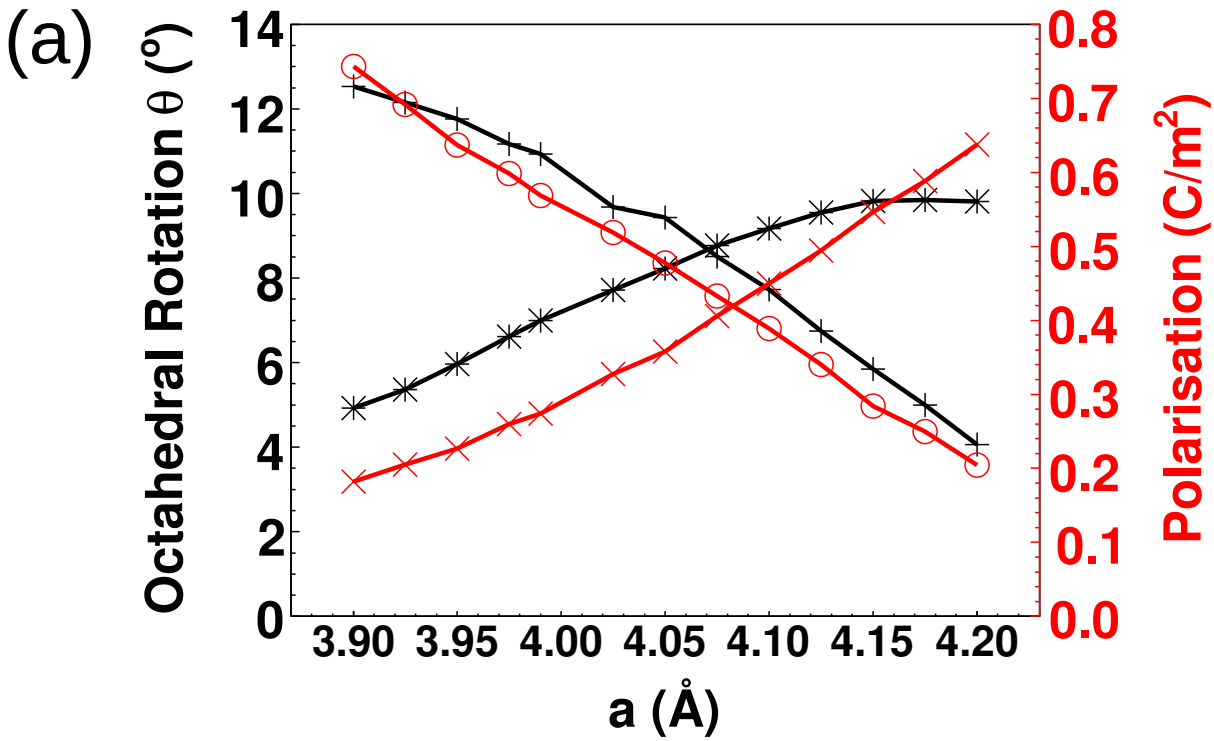
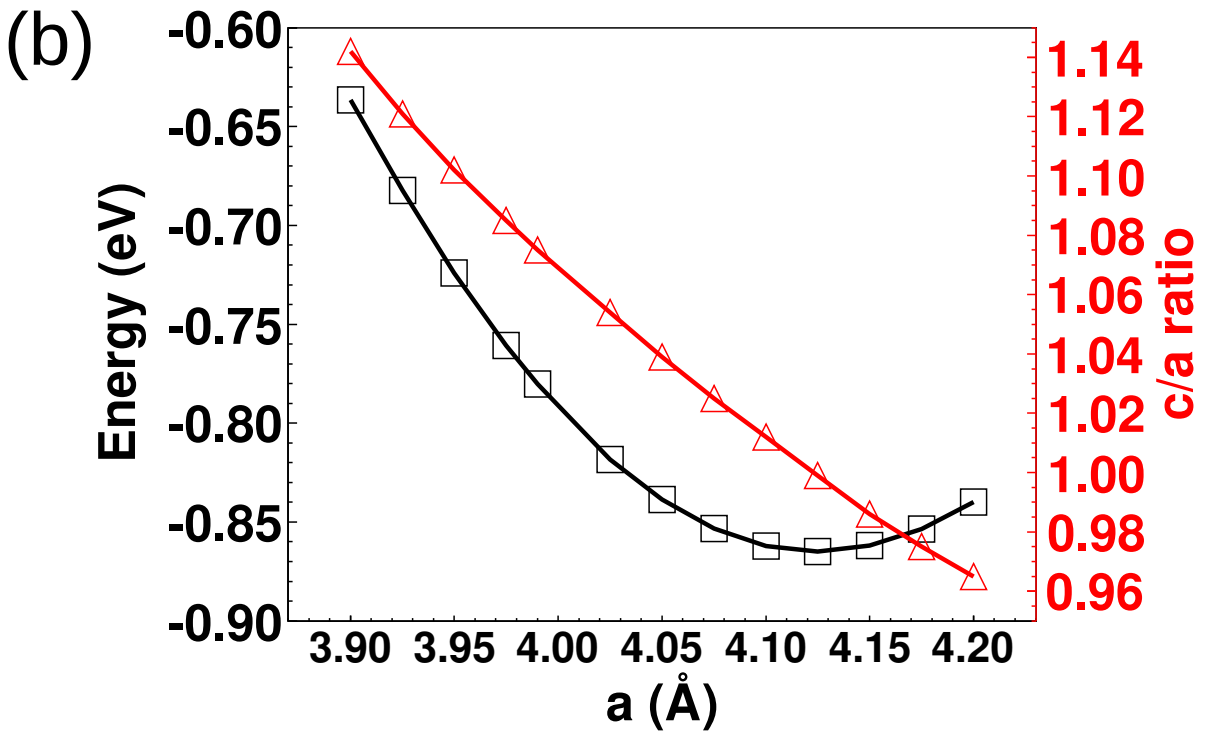

(a)
Octahedral Rotation θ (°)
Polarisation (C/m²)
a (Å)
0
2
4
6
8
10
12
14
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
3.90
3.95
4.00
4.05
4.10
4.15
4.20


(b)
Energy (eV)
c/a ratio
a (Å)
-0.60
-0.65
-0.70
-0.75
-0.80
-0.85
-0.90
1.14
1.12
1.10
1.08
1.06
1.04
1.02
1.00
0.98
0.96
3.90
3.95
4.00
4.05
4.10
4.15
4.20