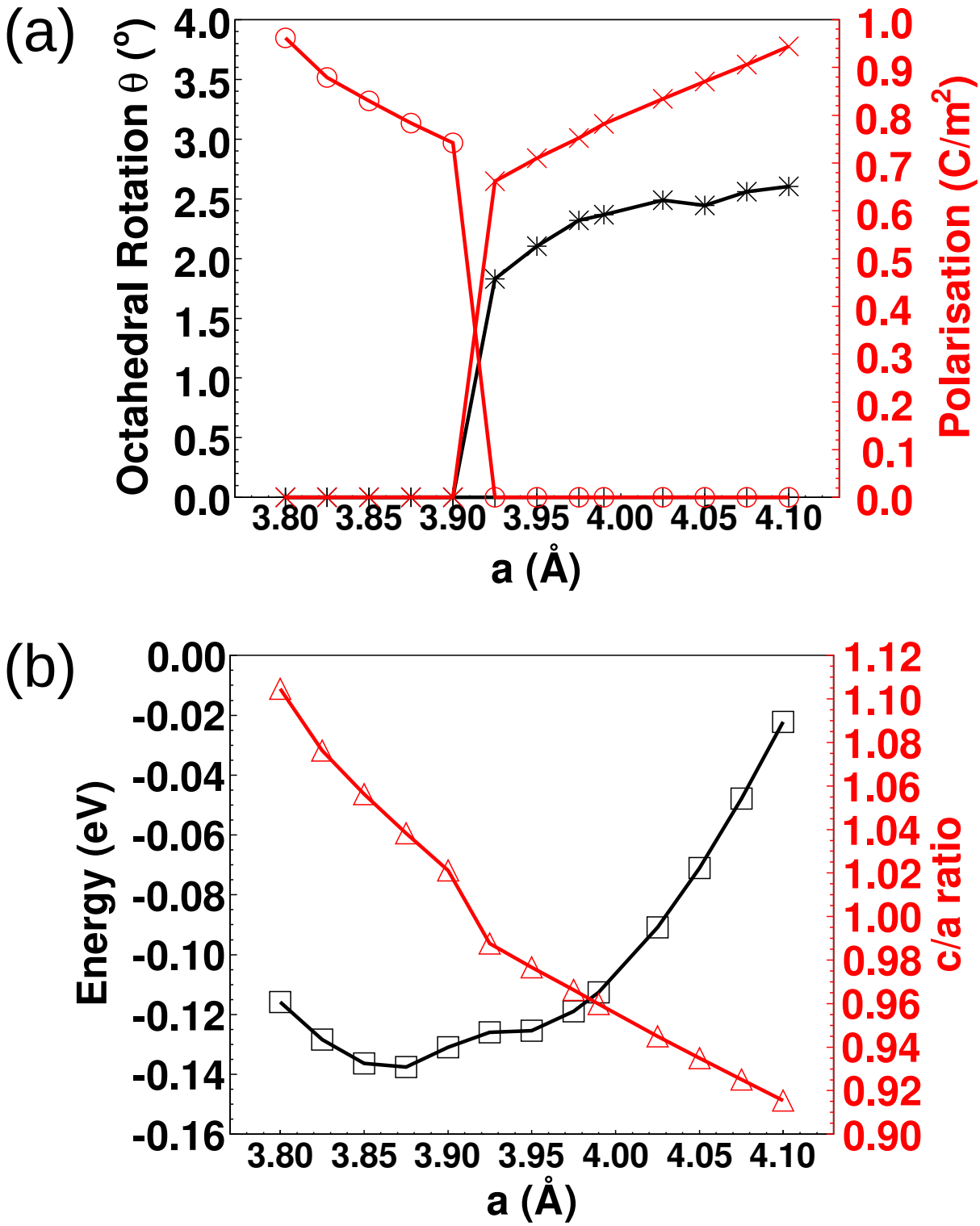
(a)
Octahedral Rotation θ (°)
Polarisation (C/m²)
a (Å)
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
3.80 3.85 3.90 3.95 4.00 4.05 4.10
(b)
Energy (eV)
c/a ratio
a (Å)
0.00
-0.02
-0.04
-0.06
-0.08
-0.10
-0.12
-0.14
-0.16
1.12
1.10
1.08
1.06
1.04
1.02
1.00
0.98
0.96
0.94
0.92
0.90
3.80 3.85 3.90 3.95 4.00 4.05 4.10