

Stoichiometric NMC811

20 % delithiated NMC811

(a) Buckingham Potential

interaction	A (eV)	ρ (Å)	C (eV·Å ⁶)
Li ⁺ ...O ²⁻	632.1018	0.2906	0.0
Ni ²⁺ ...O ²⁻	1582.50	0.2882	0.0
Co ³⁺ ...O ²⁻	1329.82	0.3087	0.0
Mn ⁴⁺ ...O ²⁻	1397.63	0.3211	0.0
O ²⁺ ...O ²⁻	22764.3	0.149	65.0

(b) Core-Shell Interaction

interaction	Y (e) (shell charge)	k (eV·Å ⁻²)
Li ⁺	1.0	9999.0
Ni ²⁺	3.344	93.7
Co ³⁺	2.04	196.3
Mn ⁴⁺	4.0	95.0
O ²⁻	-2.96	65.0

