# Electronic Supplementary Information for PCCP article

# Mechainsm of Li intercalation at the surface of $LiCoO_2$

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Basis sets details (gaussian exponents and their contraction coefficients) for Li, Co, and O atoms:

**Li**
number of radial functions
5
angular momentum, number of alphas
0 3
alphas - s - 3s/2/3s392 Eopt + reopt(c2,c1)
0.06595300d+00 0.69066600d+00 1.38140000d+00
wave function coefficients
0.08945700d+00 -0.22707000d+00 0.09077400d+00
angular momentum, number of alphas
0 1
alphas - s - second zeta s polarization
0.06595300d+00
wave function coefficients
1.00000000d+00
angular momentum, number of alphas
1 3
alphas - p - angular polarization Eopt (a,c)
0.07500000d+00 0.28000000d+00 1.22000000d+00
wave function coefficients
0.28870000d+00 0.44870000d+00 1.00000000d+00
angular momentum, number of alphas
1 1
alphas - p - angular polarization Eopt
0.07500000d+00
wave function coefficients
1.00000000d+00
angular momentum, number of alphas
2 1

alphas - p - angular polarization Eopt
0.16000000d+00
wave function coefficients
1.00000000d+00
shell occupancies for lithium Li: s(1.0)
1.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000

**Co**
number of radial functions
5
angular momentum, number of alphas
2 5
alphas - d - 5d/2/5d454 Eopt + reoptc2,c1
0.20180500d+00 0.55441400d+00 1.41387600d+00 3.82273500d+00
10.94516300d+00
wave function coefficients
0.03670400d+00 0.26293800d+00 1.77797300d+00 12.96827300d+00
-1.31161300d+00
angular momentum, number of alphas
0 4
alphas - s - 4s/2/4s392 Eopt(a2,a1,c2,c1)
0.07400000d+00 0.25000000d+00 0.81233900d+00 1.62470000d+00
wave function coefficients
0.13795000d+00 0.30040000d+00 -1.05673000d+00 0.39376000d+00
angular momentum, number of alphas
0 1
alphas - s - second zeta s polarization
0.07400000d+00
wave function coefficients
1.00000000d+00
angular momentum, number of alphas
1 2
alphas - p - angular polarization Eopt
0.12000000d+00 0.68000000d+00
wave function coefficients
1.00000000d+00 -0.66500000d+00
angular momentum, number of alphas
2 1
alphas - d - second zeta d polarization
0.20180500d+00
wave function coefficients
1.00000000d+00
shell occupancies for cobalt, Co: d(7.40)s(s1.60)
7.40000000 1.60000000 0.00000000 0.00000000 0.00000000 0.00000000

**O**
number of radial functions
5
angular momentum, number of alphas

0 5
alphas - s - 5s/2/5s284 Eopt(flat) + check (c1)
0.24022700d+00 0.68334800d+00 1.98182200d+00 3.96390000d+00
7.92780000d+00
wave function coefficients
0.33303400d+00 1.10004600d+00 1.16492600d+00 -1.95149900d+00
0.64475500d+00
angular momentum, number of alphas
1 4
alphas - p - 4p/2/4p563 Eopt + reopt(c1)
0.12928900d+00 0.40218500d+00 1.18213300d+00 3.84037500d+00
wave function coefficients
0.05931000d+00 0.37536900d+00 1.45605400d+00 3.86770800d+00
angular momentum, number of alphas
0 1
alphas - s - second zeta s polarization
0.24022700d+00
wave function coefficients
1.00000000d+00
angular momentum, number of alphas
1 1
alphas - p - second zeta p polarization
0.12928900d+00
wave function coefficients
1.00000000d+00
angular momentum, number of alphas
2 2
alphas
0.25000000d+00 1.20000000d+00
wave function coefficients
0.11720000d+00 1.00000000d+00
shell occupancies for oxygen, O s(2.0)p(4.5)p'(-0.5), -0.5 pseudoion (H2O)
2.00000000 4.50000000 0.00000000 -0.50000000 0.00000000