Supplementary Information

Machine learnt bond order potential to model metal- organic (Co-C) heterostructures

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1. Bond order potential parameters in LAMMPS format (pair/style: tersoff)

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# Tersoff parameters for various elements and mixtures
# multiple entries can be added to this file, LAMMPS reads the ones it needs
# these entries are in LAMMPS metal units:
#   A,B = eV; lambda1,lambda2,lambda3 = 1/Angstroms; R,D = Angstroms
#   other quantities are unitless

# format of a single entry (one or more lines):
#   element 1, element 2, element 3,
#   m, gamma, lambda3, c, d, costheta0, n, beta, lambda2, B, R, D, lambda1, A

Co Co Co  3 1 0 30611.5 113.064 -0.528852 0.591658 0.042649 1.34837 80.5297 3.05008
0.2 2.96998 1017.14
C C C  3 1 0 38049 4.3484 -0.57058 0.72751 1.5724e-07 2.2119 346.7 1.95 0.15 3.4879
1393.6
Co Co C   3.000000 1.000000 0 28062.2 95.0617 -0.496091 1 1 0 0.000000 2.128316
0.200000 0 0
Co C C   3.000000 1.000000 0 28062.2 95.0617 -0.496091 1 1 0.641094 36.969225 2.128316
0.200000 3.71665 585.69
Co C Co   3.000000 1.000000 0 30611.5 113.064 -0.528852 1 1 0 0.000000 3.050080
0.200000 0 0
C C Co   3.000000 1.000000 0 28062.2 95.0617 -0.496091 1 1 0 0.000000 2.128316
0.200000 0 0
C Co C   3.000000 1.000000 0 38049 4.3484 -0.570580 1 1 0 0.000000 1.950000 0.150000 0
0
C Co Co   3.000000 1.000000 0 28062.2 95.0617 -0.496091 1 1 0.641094 36.969225
2.128316 0.200000 3.71665 585.69
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