CSIRO NANOSTRUCTURE DATABANK

Header List – Gold Nanoparticle Data Set

ID	Unique identifier, filename ID.xyz
Processing Features	
T	Temperature, K
tau	Growth rate, atoms/ns
time	Time, ns
Structural Features	
N_total	Total number of atoms
N_bulk	Total number of bulk atoms
N_surface	Total number of surface atoms
Volume	Total nanoparticle volume, m^3
R_min	Nanoparticle radius minimum, Å
R_max	Nanoparticle radius maximum, Å
R_diff	Nanoparticle radius minimum, Å
R_avg	Nanoparticle radius average, Å
R_std	Nanoparticle radius standard deviation, Å
R_skew	Nanoparticle radius skewness, Å
R_kurt	Nanoparticle radius kurtosis, Å
S_100	Number of atoms located on (100) surfaces
S_111	Number of atoms located on (111) surfaces
S_110	Number of atoms located on (110) surfaces
S_311	Number of atoms located on (311) surfaces
Curve_1-10	Atoms with surface curvature angle between 1 and 10 degrees
Curve_11-20	Atoms with surface curvature angle between 11 and 20 degrees
Curve_21-30	Atoms with surface curvature angle between 21 and 30 degrees
Curve_31-40	Atoms with surface curvature angle between 31 and 40 degrees
Curve_41-50	Atoms with surface curvature angle between 41 and 50 degrees
Curve_51-60	Atoms with surface curvature angle between 51 and 60 degrees
Curve_61-70	Atoms with surface curvature angle between 61 and 70 degrees
Curve_71-80	Atoms with surface curvature angle between 71 and 80 degrees
Curve_81-90	Atoms with surface curvature angle between 81 and 90 degrees
Curve_91-100	Atoms with surface curvature angle between 91 and 100 degrees
Curve_101-110	Atoms with surface curvature angle between 101 and 110 degrees
Curve_111-120	Atoms with surface curvature angle between 111 and 120 degrees
Curve_121-130	Atoms with surface curvature angle between 121 and 130 degrees
Curve_131-140	Atoms with surface curvature angle between 131 and 140 degrees
Curve_141-150	Atoms with surface curvature angle between 141 and 150 degrees
Curve_151-160	Atoms with surface curvature angle between 151 and 160 degrees
Curve_161-170	Atoms with surface curvature angle between 161 and 170 degrees
Curve_171-180	Atoms with surface curvature angle between 171 and 180 degrees
Avg_total	Order parameters, Average coordination number of all atoms
Avg_bulk	Coordination statistics, Average coordination number of all bulk atoms
Avg_surf	Coordination statistics, Average coordination number of all surface atoms
TCN_0	Coordination statistics, Number of atoms with coordination number 0
TCN_1	Coordination statistics, Number of atoms with coordination number 1
TCN_2	Coordination statistics, Number of atoms with coordination number 2
TCN_3	Coordination statistics, Number of atoms with coordination number 3
TCN_4	Coordination statistics, Number of atoms with coordination number 4

TCN_5	Coordination statistics, Number of atoms with coordination number 5
TCN_6	Coordination statistics, Number of atoms with coordination number 6
TCN_7	Coordination statistics, Number of atoms with coordination number 7
TCN_8	Coordination statistics, Number of atoms with coordination number 8
TCN_9	Coordination statistics, Number of atoms with coordination number 9
TCN_10	Coordination statistics, Number of atoms with coordination number 10
TCN_11	Coordination statistics, Number of atoms with coordination number 11
TCN_12	Coordination statistics, Number of atoms with coordination number 12
TCN_13	Coordination statistics, Number of atoms with coordination number 13
TCN_14	Coordination statistics, Number of atoms with coordination number 14
TCN_15	Coordination statistics, Number of atoms with coordination number 15
TCN_16	Coordination statistics, Number of atoms with coordination number 16
TCN_17	Coordination statistics, Number of atoms with coordination number 17
TCN_18	Coordination statistics, Number of atoms with coordination number 18
TCN_19	Coordination statistics, Number of atoms with coordination number 19
TCN_20	Coordination statistics, Number of atoms with coordination number 20
BCN_0	Coordination statistics, Number of bulk atoms with coordination number 0
BCN_1	Coordination statistics, Number of bulk atoms with coordination number 1
BCN_2	Coordination statistics, Number of bulk atoms with coordination number 2
BCN_3	Coordination statistics, Number of bulk atoms with coordination number 3
BCN_4	Coordination statistics, Number of bulk atoms with coordination number 4
BCN_5	Coordination statistics, Number of bulk atoms with coordination number 5
BCN_6	Coordination statistics, Number of bulk atoms with coordination number 6
BCN_7	Coordination statistics, Number of bulk atoms with coordination number 7
BCN_8	Coordination statistics, Number of bulk atoms with coordination number 8
BCN_9	Coordination statistics, Number of bulk atoms with coordination number 9
BCN_10	Coordination statistics, Number of bulk atoms with coordination number 10
BCN_11	Coordination statistics, Number of bulk atoms with coordination number 11
BCN_12	Coordination statistics, Number of bulk atoms with coordination number 12
BCN_13	Coordination statistics, Number of bulk atoms with coordination number 13
BCN_14	Coordination statistics, Number of bulk atoms with coordination number 14
BCN_15	Coordination statistics, Number of bulk atoms with coordination number 15
BCN_16	Coordination statistics, Number of bulk atoms with coordination number 16
BCN_17	Coordination statistics, Number of bulk atoms with coordination number 17
BCN_18	Coordination statistics, Number of bulk atoms with coordination number 18
BCN_19	Coordination statistics, Number of bulk atoms with coordination number 19
BCN_20	Coordination statistics, Number of bulk atoms with coordination number 20
SCN_0	Coordination statistics, Number of surface atoms with coordination number 0
SCN_1	Coordination statistics, Number of surface atoms with coordination number 1
SCN_2	Coordination statistics, Number of surface atoms with coordination number 2
SCN_3	Coordination statistics, Number of surface atoms with coordination number 3
SCN_4	Coordination statistics, Number of surface atoms with coordination number 4
SCN_5	Coordination statistics, Number of surface atoms with coordination number 5
SCN_6	Coordination statistics, Number of surface atoms with coordination number 6
SCN_7	Coordination statistics, Number of surface atoms with coordination number 7
SCN_8	Coordination statistics, Number of surface atoms with coordination number 8
SCN_9	Coordination statistics, Number of surface atoms with coordination number 9
SCN_10	Coordination statistics, Number of surface atoms with coordination number 10
SCN_11	Coordination statistics, Number of surface atoms with coordination number 11
SCN_12	Coordination statistics, Number of surface atoms with coordination number 12
SCN_13	Coordination statistics, Number of surface atoms with coordination number 13
SCN_14	Coordination statistics, Number of surface atoms with coordination number 14

SCN_15	Coordination statistics, Number of surface atoms with coordination number 15
SCN_16	Coordination statistics, Number of surface atoms with coordination number 16
SCN_17	Coordination statistics, Number of surface atoms with coordination number 17
SCN_18	Coordination statistics, Number of surface atoms with coordination number 18
SCN_19	Coordination statistics, Number of surface atoms with coordination number 19
SCN_20	Coordination statistics, Number of surface atoms with coordination number 20
Avg_bonds	Bonding statistics, Average bond length, Å
Std_bonds	Bonding statistics, Standard Deviation of the bond length, Å
Max_bonds	Bonding statistics, Maximum bond length, Å
Min_bonds	Bonding statistics, Minimum bond length, Å
N_bonds	Bonding statistics, Total number of bonds
angle_avg	Bonding statistics, Average bond angle, Degrees
angle_std	Bonding statistics, Standard deviations of the bond angle, Degrees
FCC	Lattice statistics, Number of atoms in face centred cubic (fcc) lattice
HCP	Lattice statistics, Number of atoms in hexagonal closed packed (hcp) lattice
ICOS	Lattice statistics, Number of atoms in icosahedral lattice
DECA	Lattice statistics, Number of atoms in decahedral lattice
q6q6_avg_total	Order parameters, Average spherical harmonic (q6.q6 >0.7) for all atoms
q6q6_avg_bulk	Order parameters, Average spherical harmonic (q6.q6 >0.7) for all bulk atoms
q6q6_avg_surf	Order parameters, Average spherical harmonic (q6.q6 >0.7) for all surface atoms
q6q6_T0	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 0
q6q6_T1	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 1
q6q6_T2	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 2
q6q6_T3	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 3
q6q6_T4	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 4
q6q6_T5	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 5
q6q6_T6	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 6
q6q6_T7	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 7
q6q6_T8	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 8
q6q6_T9	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 9
q6q6_T10	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 10
q6q6_T11	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 11
q6q6_T12	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 12
q6q6_T13	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 13
q6q6_T14	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 14
q6q6_T15	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 15
q6q6_T16	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 16
q6q6_T17	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 17
q6q6_T18	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 18
q6q6_T19	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 19
q6q6_T20	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) of 20
q6q6_T20+	Order parameters, Number of atoms with spherical harmonic (q6.q6 >0.7) greater than 20
q6q6_B0	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 0
q6q6_B1	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 1
q6q6_B2	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 2
q6q6_B3	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 3
q6q6_B4	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 4
q6q6_B5	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 5
q6q6_B6	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 6
q6q6_B7	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 7
q6q6_B8	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 8
q6q6_B9	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 9

q6q6_B10	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 10
q6q6_B11	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 11
q6q6_B12	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 12
q6q6_B13	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 13
q6q6_B14	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 14
q6q6_B15	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 15
q6q6_B16	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 16
q6q6_B17	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 17
q6q6_B18	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 18
q6q6_B19	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 19
q6q6_B20	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) of 20
q6q6_B20+	Order parameters, Number of bulk atoms with spherical harmonic (q6.q6 >0.7) greater than 20
q6q6_S0	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 0
q6q6_S1	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 1
q6q6_S2	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 2
q6q6_S3	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 3
q6q6_S4	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 4
q6q6_S5	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 5
q6q6_S6	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 6
q6q6_S7	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 7
q6q6_S8	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 8
q6q6_S9	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 9
q6q6_S10	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 10
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q6q6_S12	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 12
q6q6_S13	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 13
q6q6_S14	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 14
q6q6_S15	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 15
q6q6_S16	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 16
q6q6_S17	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 17
q6q6_S18	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 18
q6q6_S19	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 19
q6q6_S20	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) of 20
q6q6_S20+	Order parameters, Number of surface atoms with spherical harmonic (q6.q6 >0.7) greater than 20

Target Property Labels

Total_E	Total energy of the nanoparticle from the LAMMPS simulation, eV
Formation_E	Formation energy of the nanoparticle (Total_E- N_total*Bulk_E/atom), eV Where the Bulk_E/atom is provided on the website for the EAM potential