CSIRO NANOSTRUCTURE DATABANK

Header List – Silver Nanoparticle Data Set

ID	File name and unique identifier
Structural Features	
Shape	The zonohedron of the polyhedral nanoparticle
N_Atoms	Total number of atoms
N_Bulk	Total number of bulk atoms
N_Surface	Total number of surface atoms
R_min	Minimum radius, in Å
R_max	Maximum radius, in Å
R_diff	Difference between minimum and maximum radius, in Å
R_avg	Average radius, in Å
R_std	Standard deviation of the radius, in Å
R_skew	Skewness of the radius, in Å
R_kurt	Kurtosis of the radius, in Å
Anisotropy	Aspect ratio
S_100	Number of atoms on (100) surface facet
S_111	Number of atoms on (111) surface facet
S_110	Number of atoms on (110) surface facet
S_311	Number of atoms on (311) surface facet
N_facets	Number of surface facets
Curve_0-10	Surface curvature angle between 1 and 10 degrees
Curve_11-20	Surface curvature angle between 11 and 20 degrees
Curve_21-30	Surface curvature angle between 21 and 30 degrees
Curve_31-40	Surface curvature angle between 31 and 40 degrees
Curve_41-50	Surface curvature angle between 41 and 50 degrees
Curve_51-60	Surface curvature angle between 51 and 60 degrees
Curve_61-70	Surface curvature angle between 61 and 70 degrees
Curve_71-80	Surface curvature angle between 71 and 80 degrees
Curve_81-90	Surface curvature angle between 81 and 90 degrees
Curve_91-100	Surface curvature angle between 91 and 100 degrees
Curve_101-110	Surface curvature angle between 101 and 110 degrees
Curve_111-120	Surface curvature angle between 111 and 120 degrees
Curve_121-130	Surface curvature angle between 121 and 130 degrees
Curve_131-140	Surface curvature angle between 131 and 140 degrees
Curve_141-150	Surface curvature angle between 141 and 150 degrees
Curve_151-160	Surface curvature angle between 151 and 160 degrees
Curve_161-170	Surface curvature angle between 161 and 170 degrees
Curve_171-180	Surface curvature angle between 171 and 180 degrees
Avg_total	Coordination statistics, average Ag coordination number
Avg_bulk	Coordination statistics, average bulk Ag coordination number
Avg_surf	Coordination statistics, average surface Ag coordination number
SCN1	Degree of under-coordination number of surface atoms, surface coordination number 1
SCN2	Degree of under-coordination number of surface atoms, surface coordination number 2
SCN3	Degree of under-coordination number of surface atoms, surface coordination number 3
SCN4	Degree of under-coordination number of surface atoms, surface coordination number 4
SCN5	Degree of under-coordination number of surface atoms, surface coordination number 5

SCN6	Degree of under-coordination number of surface atoms, surface coordination number 6
SCN7	Degree of under-coordination number of surface atoms, surface coordination number 7
SCN8	Degree of under-coordination number of surface atoms, surface coordination number 8
SCN9	Degree of under-coordination number of surface atoms, surface coordination number 9
SCN10	Degree of under-coordination number of surface atoms, surface coordination number 10
SCN11	Degree of under-coordination number of surface atoms, surface coordination number 11
SCN12	Degree of under-coordination number of surface atoms, surface coordination number 12
Avg	Average Ag-Ag bond length, in Å
Std_dev	Standard deviations of the Ag-Ag bond length, in Å
Max	Maximum Ag-Ag bond length, in Å
Min	Minimum Ag-Ag bond length, in Å
N_Bonds	Total number of Ag-Ag bonds
FCC	Total number of FCC atoms
HCP	Total number of HCP atoms
ICOS	Total number of ICOS atoms
DECA	Total number of DECA atoms
Avg_total	Spherical harmonics q6.q6 > 0.7 coordination, average order parameter
Avg_bulk	Spherical harmonics q6.q6 > 0.7 coordination, average order parameter of bulk atoms
Avg_surf	Spherical harmonics q6.q6 > 0.7 coordination, average order parameter or surface atoms
T0	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 0
T1	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 1
T2	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 2
T3	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 3
T4	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 4
T5	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 5
T6	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 6
T7	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 7
T8	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 8
T9	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 9
T10	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 10
T11	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11
T12	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12
T13	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13
T14	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14
T15	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15
T16	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16
T17	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17
T18	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18
T19	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19
T20	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20
T>20	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20
Target Property Labels	
Formation_E	Formation energy, (E_np-E_bulk)/N_atoms, in eV
EF	Energy of the Fermi level, in eV
IP	Ionisation potential, in eV
EA	Electron affinity, in eV
EG	Electronic band gap, in eV