CSIRO NANOSTRUCTURE DATABANK

Header List – PdCo Nanoparticle Data Set

ID	Unique identifier, filename being ID.xyz
Processing Features	
T	Temperature, K
P	Pressure, bars
Structural Features	
N_atom_total	Total number of atoms
N_{Ele}	Total number of atoms with element type {Ele}
N_atom_bulk	Total number of bulk atoms
N_atom_surface	Total number of surface atoms
Vol_bulk_pack	Nanoparticle volume, assuming bulk packing, Å
Vol_sphere	Nanoparticle volume, assuming spherical shape with radius R_avg, Å
R_min	Minimum nanoparticle radius, Å
R_max	Maximum nanoparticle radius, Å
R_diff	Difference between maximum and minimum nanoparticle radii, Å
R_avg	Average nanoparticle radius, Å
R_std	Nanoparticle radius standard deviation, Å
R_skew	Nanoparticle radius skewness
R_kurt	Nanoparticle radius kurtosis
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_{i}	Number of atoms with surface curvature angle of {i} degree
MM_TCN_avg	Coordination statistics, Average coordination number of all atoms
MM_BCN_avg	Coordination statistics, Average coordination number of bulk atoms
MM_SCN_avg	Coordination statistics, Average coordination number of surface atoms
MM_SOCN_avg	Coordination statistics, Average surface-only coordination number of surface atoms
MM_TGCN_avg	Coordination statistics, Average generalised coordination number of all atoms
MM_BGCN_avg	Coordination statistics, Average generalised coordination number of bulk atoms
MM_SGCN_avg	Coordination statistics, Average generalised coordination number of surface atoms
MM_SOGCN_avg	Coordination statistics, Average surface-only generalised coordination number of surface atoms
MM_TCN_{i}	Coordination statistics, Number of atoms with coordination number {i}
MM_BCN_{i}	Coordination statistics, Number of bulk atoms with coordination number {i}
MM_SCN_{i}	Coordination statistics, Number of surface atoms with coordination number {i}
MM_SOCN_{i}	Coordination statistics, Number of surface atoms with surface-only coordination number {i}
MM_TGCN_{i}	Coordination statistics, Number of atoms with generalised coordination number {i}
MM_BGCN_{i}	Coordination statistics, Number of bulk atoms with generalised coordination number {i}
MM_SGCN_{i}	Coordination statistics, Number of surface atoms with generalised coordination number {i}
MM_SOGCN_{i}	Coordination statistics, Number of surface atoms with surface-only generalised coordination number {i}
{Ele}M_TCN_avg	Coordination statistics, Average coordination number of all {Ele} atoms
{Ele}M_BCN_avg	Coordination statistics, Average coordination number of bulk {Ele} atoms
{Ele}M_SCN_avg	Coordination statistics, Average coordination number of surface {Ele} atoms
{Ele}M_SOCN_avg	Coordination statistics, Average surface-only coordination number of surface {Ele} atoms
{Ele}M_TGCN_avg	Coordination statistics, Average generalised coordination number of all {Ele} atoms
{Ele}M_BGCN_avg	Coordination statistics, Average generalised coordination number of bulk {Ele} atoms
{Ele}M_SGCN_avg	Coordination statistics, Average generalised coordination number of surface {Ele} atoms
{Ele}M_SOGCN_avg	Coordination statistics, Average surface-only generalised coordination number of surface {Ele} atoms
{Ele}M_TCN_{i}	Coordination statistics, Number of {Ele} atoms with coordination number {i}
{Ele}M_BCN_{i}	Coordination statistics, Number of bulk {Ele} atoms with coordination number {i}
{Ele}M_SCN_{i}	Coordination statistics, Number of surface {Ele} atoms with coordination number {i}
{Ele}M_SOCN_{i}	Coordination statistics, Number of surface {Ele} atoms with surface-only coordination number {i}
{Ele}M_TGCN_{i}	Coordination statistics, Number of {Ele} atoms with generalised coordination number {i}
{Ele}M_BGCN_{i}	Coordination statistics, Number of bulk {Ele} atoms with generalised coordination number {i}
{Ele}M_SGCN_{i}	Coordination statistics, Number of surface {Ele} atoms with generalised coordination number {i}

{Ele}M_SOGCN_{i}	Coordination statistics, Number of surface {Ele} atoms with surface-only generalised coordination number {i}
MM_BL_avg	Bonding statistics, Average bond length for all atoms, Å
MM_BL_std	Bonding statistics, Standard deviation of bond lengths for all atoms, Å
MM_BL_max	Bonding statistics, Maximum bond length among all atoms, Å
MM_BL_min	Bonding statistics, Minimum bond length among all atoms, Å
MM_BL_num	Bonding statistics, Total number of bonds in nanoparticle
{Ele1}{Ele2}_BL_avg	Bonding statistics, Average {Ele1}-{Ele2} bond length, Å
{Ele1}{Ele2}_BL_std	Bonding statistics, Standard deviation of {Ele1}-{Ele2} bond lengths, Å
{Ele1}{Ele2}_BL_max	Bonding statistics, Maximum {Ele1}-{Ele2} bond length, Å
{Ele1}{Ele2}_BL_min	Bonding statistics, Minimum {Ele1}-{Ele2} bond length, Å
{Ele1}{Ele2}_BL_num	Bonding statistics, Total number of {Ele1}-{Ele2} bonds
{Ele1}{Ele2}_frac	Bonding statistics, Fraction of {Ele1}-{Ele2} bonds
MMM_BA1_avg	Bonding statistics, Average first-order bond angle for all atoms, Degrees
MMM_BA1_std	Bonding statistics, Standard deviation of first-order bond angles for all atoms, Degrees
MMM_BA1_max	Bonding statistics, Maximum first-order bond angle for all atoms, Degrees
MMM_BA1_min	Bonding statistics, Minimum first-order bond angle for all atoms, Degrees
MMM_BA1_num	Bonding statistics, Total number of first-order bond angles for all atoms
{Ele1}{Ele2}{Ele3}_BA1_avg	Bonding statistics, Average first-order {Ele1}-{Ele2}-{Ele3} bond angle, Degrees
{Ele1}{Ele2}{Ele3}_BA1_std	Bonding statistics, Standard deviation of first-order {Ele1}-{Ele2}-{Ele3} bond angles, Degrees
{Ele1}{Ele2}{Ele3}_BA1_max	Bonding statistics, Maximum first-order {Ele1}-{Ele2}-{Ele3} bond angle, Degrees
{Ele1}{Ele2}{Ele3}_BA1_min	Bonding statistics, Minimum first-order {Ele1}-{Ele2}-{Ele3} bond angle, Degrees
{Ele1}{Ele2}{Ele3}_BA1_num	Bonding statistics, Total number of first-order {Ele1}-{Ele2}-{Ele3} bond angles
MMM_BA2_avg	Bonding statistics, Average second-order bond angle for all atoms, Degrees
MMM_BA2_std	Bonding statistics, Standard deviation of second-order bond angles for all atoms, Degrees
MMM_BA2_max	Bonding statistics, Maximum second-order bond angle for all atoms, Degrees
MMM_BA2_min	Bonding statistics, Minimum second-order bond angle for all atoms, Degrees
MMM_BA2_num	Bonding statistics, Total number of second-order bond angles for all atoms
{Ele1}{Ele2}{Ele3}_BA2_avg	Bonding statistics, Average second-order {Ele1}-{Ele2}-{Ele3} bond angle, Degrees
{Ele1}{Ele2}{Ele3}_BA2_std	Bonding statistics, Standard deviation of second-order {Ele1}-{Ele2}-{Ele3} bond angles, Degrees
{Ele1}{Ele2}{Ele3}_BA2_max	Bonding statistics, Maximum second-order {Ele1}-{Ele2}-{Ele3} bond angle, Degrees
{Ele1}{Ele2}{Ele3}_BA2_min	Bonding statistics, Minimum second-order {Ele1}-{Ele2}-{Ele3} bond angle, Degrees
{Ele1}{Ele2}{Ele3}_BA2_num	Bonding statistics, Total number of second-order {Ele1}-{Ele2}-{Ele3} bond angles
MMMM_BTneg_avg	Bonding statistics, Average negative dihedral angle for all atoms, Degrees
MMMM_BTneg_std	Bonding statistics, Standard deviation of negative dihedral angles for all atoms, Degrees
MMMM_BTneg_max	Bonding statistics, Maximum negative dihedral angle for all atoms, Degrees
MMMM_BTneg_min	Bonding statistics, Minimum negative dihedral angle for all atoms, Degrees
MMMM_BTneg_num	Bonding statistics, Total number of negative dihedral angles for all atoms
MMMM_BTpos_avg	Bonding statistics, Average positive dihedral angle for all atoms, Degrees
MMMM_BTpos_std	Bonding statistics, Standard deviation of positive dihedral angles for all atoms, Degrees
MMMM_BTpos_max	Bonding statistics, Maximum positive dihedral angle for all atoms, Degrees
MMMM_BTpos_min	Bonding statistics, Minimum positive dihedral angle for all atoms, Degrees
MMMM_BTpos_num	Bonding statistics, Total number of positive dihedral angles for all atoms
{Ele1}{Ele2}{Ele3}{Ele4}_BTneg_avg	Bonding statistics, Average negative {Ele1}-{Ele2}-{Ele3}-{Ele4} dihedral angle, Degrees
{Ele1}{Ele2}{Ele3}{Ele4}_BTneg_std	Bonding statistics, Standard deviation of negative {Ele1}-{Ele2}-{Ele3}-{Ele4} dihedral angles, Degrees
{Ele1}{Ele2}{Ele3}{Ele4}_BTneg_max	Bonding statistics, Maximum negative {Ele1}-{Ele2}-{Ele3}-{Ele4} dihedral angle, Degrees
{Ele1}{Ele2}{Ele3}{Ele4}_BTneg_min	Bonding statistics, Minimum negative {Ele1}-{Ele2}-{Ele3}-{Ele4} dihedral angle, Degrees

{Ele1}{Ele2}{Ele3}{Ele4}_BTneg_num	Bonding statistics, Total number of negative {Ele1}-{Ele2}-{Ele3}-{Ele4} dihedral angles
{Ele1}{Ele2}{Ele3}{Ele4}_BTpos_avg	Bonding statistics, Average positive {Ele1}-{Ele2}-{Ele3}-{Ele4} dihedral angle, Degrees
{Ele1}{Ele2}{Ele3}{Ele4}_BTpos_std	Bonding statistics, Standard deviation of positive {Ele1}-{Ele2}-{Ele3}-{Ele4} dihedral angles, Degrees
{Ele1}{Ele2}{Ele3}{Ele4}_BTpos_max	Bonding statistics, Maximum positive {Ele1}-{Ele2}-{Ele3}-{Ele4} dihedral angle, Degrees
{Ele1}{Ele2}{Ele3}{Ele4}_BTpos_min	Bonding statistics, Minimum positive {Ele1}-{Ele2}-{Ele3}-{Ele4} dihedral angle, Degrees
{Ele1}{Ele2}{Ele3}{Ele4}_BTpos_num	Bonding statistics, Total number of positive {Ele1}-{Ele2}-{Ele3}-{Ele4} dihedral angles
q6q6_T_avg	Order parameters, Average spherical harmonic (q6.q6 > 0.7) for all atoms
q6q6_B_avg	Order parameters, Average spherical harmonic (q6.q6 > 0.7) for all bulk atoms
q6q6_S_avg	Order parameters, Average spherical harmonic (q6.q6 > 0.7) for all surface atoms
q6q6_T_{i}	Order parameters, Number of atoms with spherical harmonic (q6·q6 > 0.7) of {i}
q6q6_T_20+	Order parameters, Number of atoms with spherical harmonic (q6·q6 > 0.7) greater than 20
q6q6_B_{i}	Order parameters, Number of bulk atoms with spherical harmonic (q6·q6 > 0.7) of {i}
q6q6_B_20+	Order parameters, Number of bulk atoms with spherical harmonic (q6·q6 > 0.7) greater than 20
q6q6_S_{i}	Order parameters, Number of surface atoms with spherical harmonic (q6·q6 > 0.7) of {i}
q6q6_S_20+	Order parameters, Number of surface atoms with spherical harmonic (q6·q6 > 0.7) greater than 20
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
Target Property Labels	
Total_E	Total energy of the nanoparticle from LAMMPS simulation, eV
Formation_E	Formation energy of the nanoparticle, calculated from the formula ***Total_E-(N_Pd*Pd_Bulk_E_per_atom + N_Co*Co_Bulk_E_per_atom)***, the values of ***Pd_Bulk_E_per_atom*** and ***Co_Bulk_E_per_atom*** are provided on the website from which the EAM potential was obtained, eV

[1]Surface-only coordination numbers are calculated by considering only surface atoms as neighbouring atoms.

[2]A generalised coordination number is calculated by including information about the 2nd nearest neighbours of an atom, more information could be found at Calle-Vallejo, F., Martínez, J.I., García-Lastra, J.M., Sautet, P. and Loffreda, D. (2014), Fast Prediction of Adsorption Properties for Platinum Nanocatalysts with Generalized Coordination Numbers. Angew. Chem. Int. Ed., 53: 8316-8319. https://doi.org/10.1002/anie.201402958.

[3]A first order bond angle of an atom is defined here as the angle between two of its first nearest neighbours, with the atom being the vertex.

[4]A second order bond angle of an atom is defined here as the angle between the atom and one of its second nearest neighbours, with one of its first nearest neighbour being the vertex.