

ID: Unique Identification Name, corresponding to the *.xyz molecular structure file

geom Label:

- 1: CO (cuboctahedron)
- 2: DH (the decahedron)
- 3: GRC (great rhombicuboctahedron)
- 4: HO (hexakis octahedron)
- 5: IH (icosahedron)
- 6: TC (truncated cube)
- 7: RD (rhombic dodecahedron)
- 8: mTO (modified truncated octahedron)
- 9: OH (octahedron)
- 10: RH (truncated rhombic dodecahedron)
- 11: RO (rhombi-truncated octahedron)
- 12: SRC (small rhombicuboctahedron)
- 13: T (tetrahedron)
- 14: TH (tetrakis hexahedron)
- 15: TO (truncated octahedron)
- 16: TR (triaxis octahedron)
- 17: TZ (trapezohedron)

number of Ag atoms: total number of Ag atoms in the structure

mass density ($\text{g}\cdot\text{cm}^{-3}$): mass density of the Ag nanoparticle

volume per atom ($\text{\AA}^3/\text{atom}$): averaged volume occupied by each atom

particle density (cm^{-3}): number of particles in unit volume

Ag-Ag-coordinate number: average Ag-Ag atoms coordinate number of first neighbours

mean value (Bond Ag-Ag): mean Ag-Ag bond length

error (Bond Ag-Ag): Ag-Ag bond length variance

total number (Bond Ag-Ag): total number of Ag-Ag bond

mean value (Angle Ag-Ag-Ag): mean Ag-Ag-Ag bond angle

error (Angle Ag-Ag-Ag): Ag-Ag-Ag bond angle variance

total number (Angle Ag-Ag-Ag): total number of Ag-Ag-Ag angle

number of surface atoms: total number Ag atoms on the surface

average diameter (nm): spherically averaged diameter in nm

aspect ratio: the ratio of the longest diameter and the shortest diameter

fcc population: relative number of atoms in Face-Centred Cubic (FCC) system

hcp population: relative number of atoms in Hexagonal Close Packed (HCP) system

icosahedral population: relative number of atoms in Icosahedral system

SCN1~12: relative number of surface atoms with Surface Coordinate Number (SCN) 1 to 12

Fermi energy (eV): the energy of Fermi level

Ionisation Potential (eV): the energy of Ionisation Potential, IP (eV)

Electron Affinity (eV): the electron affinity, EA (eV)

Band Gap (eV): the electronic band gap (eV)