SUPPLEMENTARY INFORMATION

Silica-induced electron loss of silver nanoparticles

Magali Benoit*[a], Joël Puibasset[b], Caroline Bonafos[a] and Nathalie Tarrat*[a]

1 Transformation of Ag_{55}

Figure S1 shows the transformation into an icosahedron when the Ag_{55} is initially in the cuboctahedral morphology. For clarity, the silica matrix has been removed.

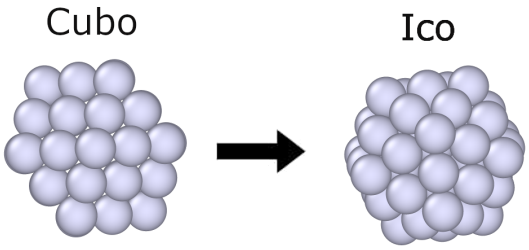

Figure S1: Transformation of an Ag_{55} cuboctahedron into an icosahedron during the relaxation. The silica matrix is not shown.

2 Structure of silica

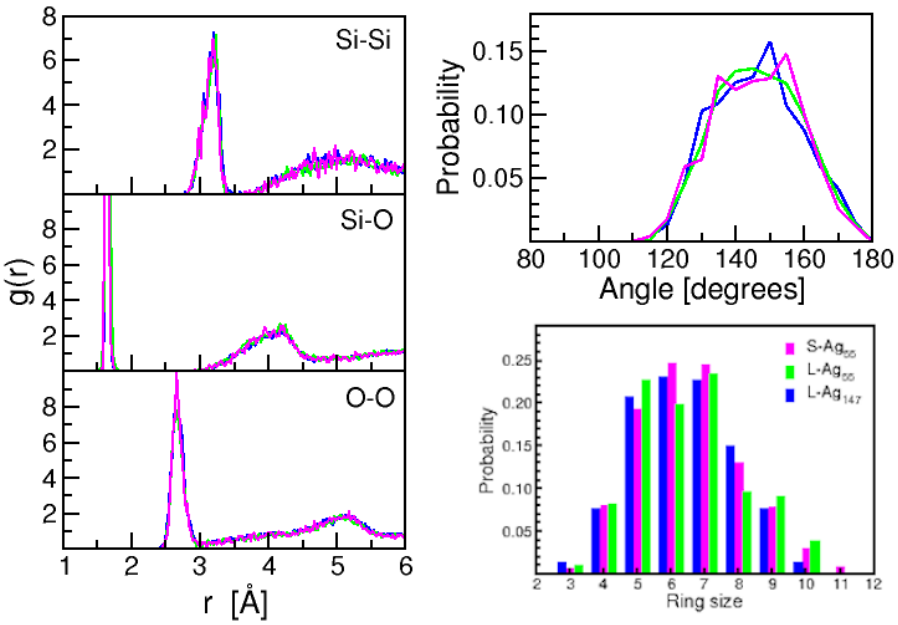

Figure S2: Comparison of the radial distribution functions g(r), of the Si-O-Si angular distribution and of the ring size statistics for L-Ag_{147}, L-Ag_{55} and S-Ag_{55}.

3 Relaxation of the systems

The following figures (Figs. S3, S4, S5) present the evolution of the total energy as a function of the relaxation steps. For L-Ag_{147} and L*-Ag_{147}, the relaxations have been carried out in several steps during which only a subset of the atoms were allowed to relax. For all systems, the first part of the relaxation was performed with a low energy cutoff (ENCUT) of 300 eV and followed by a 500 eV energy cutoff relaxation.

The coloring code in the images corresponds to the displacement of atoms during the corresponding relaxation part. No images are shown if the displacements were lower than 0.05 Å .

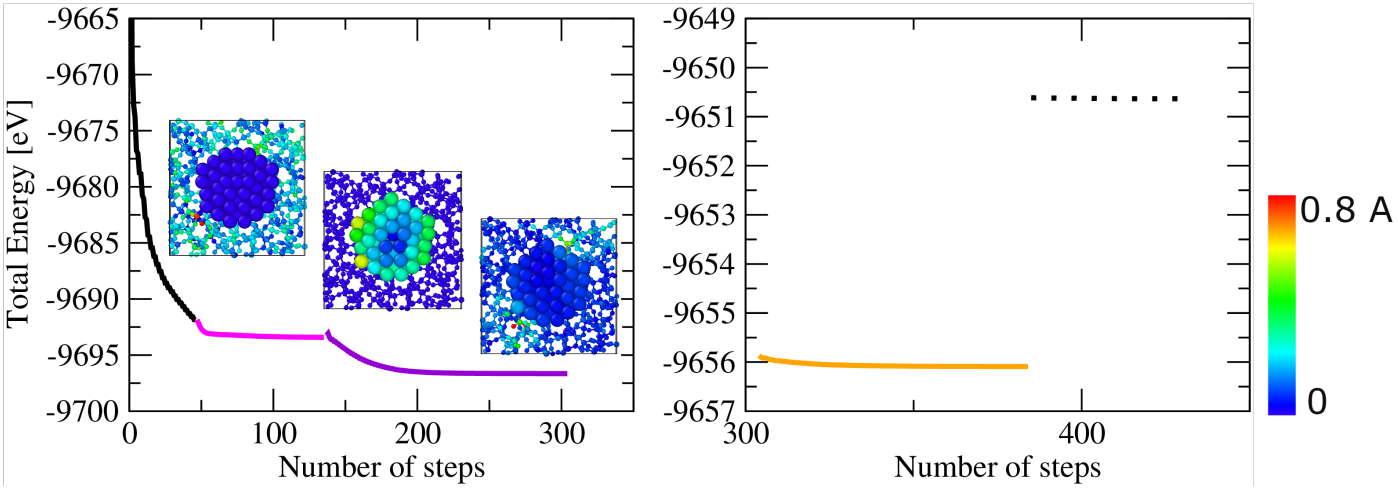

Figure S3: Total energy as a function of the relaxation steps for L-Ag_{147}. Black: only Si and O atoms are free to move, ENCUT = 300 eV. Magenta: only Ag atoms are free to move, ENCUT = 300 eV. Purple : All atoms are free to move, ENCUT = 300 eV. Orange: all atoms are free to move, ENCUT = 500 eV. Dotted black: All atoms are free to move, ENCUT = 500 eV, VASP Precision mode = Accurate. In the images, the atoms are colored as a function of their displacement during the corresponding relaxation (the color bar indicates the scale).

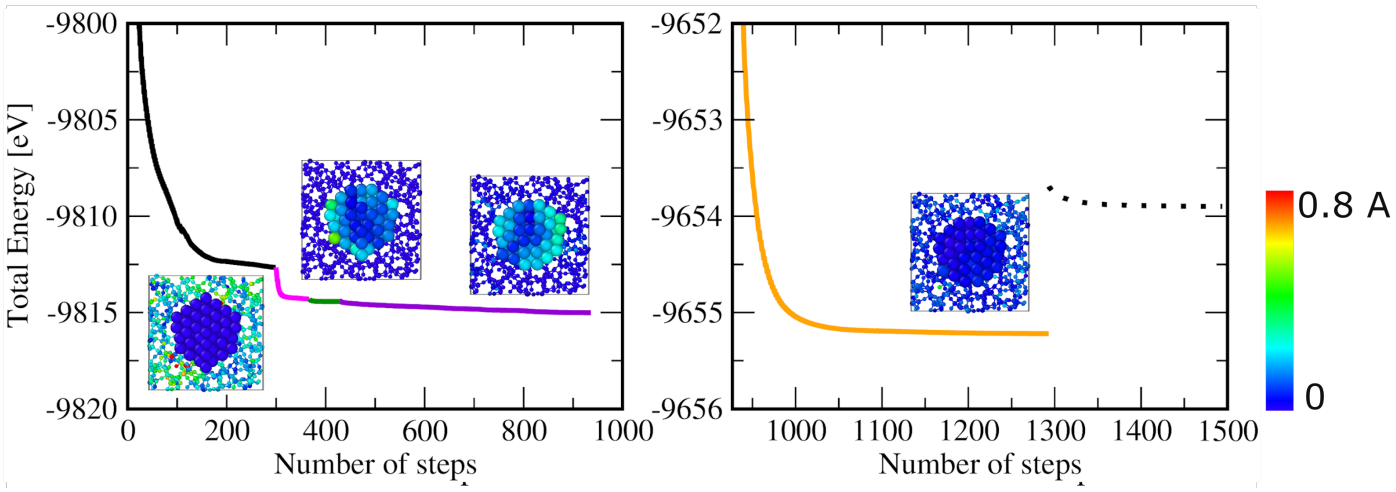

Figure S4: Total energy as a function of the relaxation steps for L*-Ag_{147}. Black: only Si and O atoms are free to move, ENCUT = 300 eV. Magenta: only Ag atoms are free to move, ENCUT = 300 eV. Green: only interface atoms are free to move, ENCUT = 300 eV. Purple : All atoms are free to move, ENCUT = 300 eV. Orange: All atoms are free to move, ENCUT = 500 eV. Dotted black: All atoms are free to move, ENCUT = 500 eV, VASP Precision mode = Accurate. In the images, the atoms are colored as a function of their displacement during the corresponding relaxation (the color bar indicates the scale).

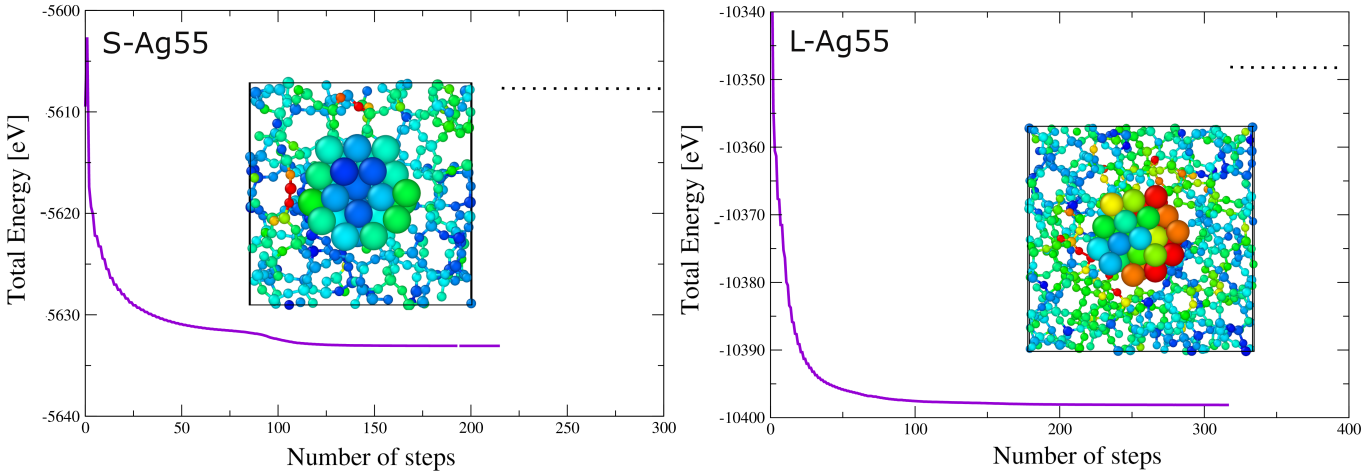

Figure S5: Total energy as a function of the relaxation steps for S-Ag_{55} and L-Ag_{55}. Purple : All atoms are free to move, ENCUT = 300 eV. Dotted black: All atoms are free to move, ENCUT = 500 eV, VASP Precision mode = Accurate. In the images, the atoms are colored as a function of their displacement during the corresponding relaxation (the color bar indicates the scale).

4 Ag charges as a function of Ag-O and Ag-Si distances

Figure S6 presents the correlation between the charge bear by the Ag atoms in L-Ag_{147} and their shortest distance to the O and Si atoms of the silica matrix.

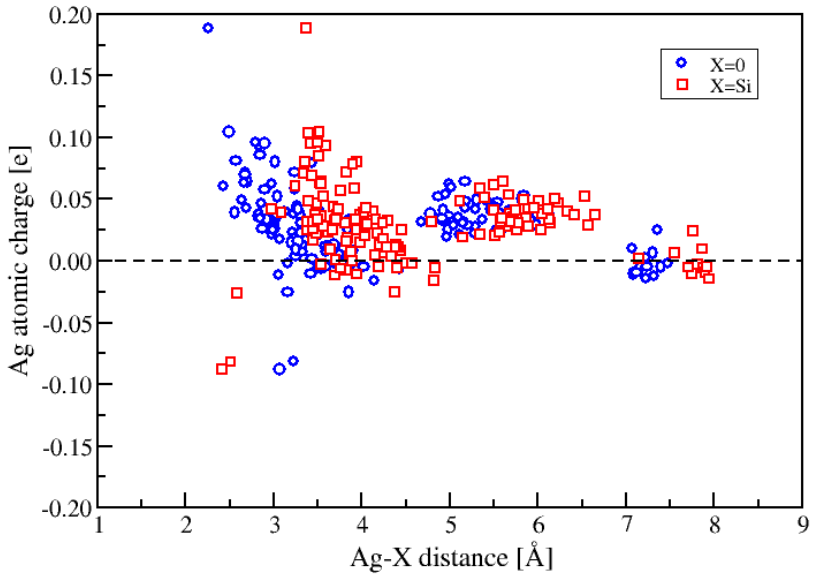

Figure S6: Atomic charges on Ag as a function of their shortest distances to the O and Si atoms, respectively.