

Supporting Information

Optical properties of size selected neutral Ag clusters: electronic shell structures and the surface plasmon resonance

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DFT calculations have been performed using the exchange and correlation functional ω B97x¹ and a relativistic effective core potential (RECP), so that only 19 electrons per atom were treated explicitly, together with the corresponding Gaussian basis set^{2,3}. The geometrical structures of Ag_n have been taken from a study by Chen *et al.*⁴ using a genetic algorithm with an embedded atom method potential, except that of Ag₂₀ which has been taken as the ground state structure of C_s symmetry obtained with DFT⁵. Calculations have been performed with the Gaussian09 suite of programs⁶.

The three figures **S1**, **S2**, **S3** give the density of states (DOS) together with the Kohn-Sham orbitals of valence orbitals for Ag₂₀, Ag₅₅ and Ag₉₂. The s-type valence electrons are found to be distributed in the following energy sequence of electronic shell model 1S², 1P⁶, 1D¹⁰, 2S², 1F¹⁴, 2P⁶, 1G¹⁸, 2D¹⁰, 3S², 1H²². We can easily distinguish the orbitals associated to S, P, D, F, G supershells. Some shells are splitting into subshells due to the lower symmetry with respect to the K_n group for a perfect sphere, and the atomic structure.

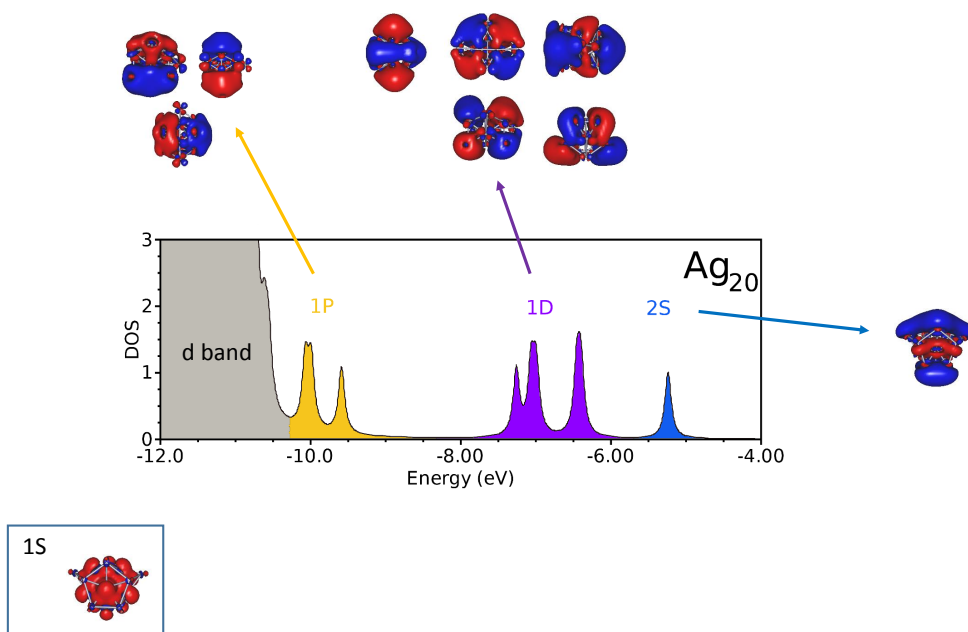


Figure S1: Density of states of Ag₂₀ together with the representative Kohn-Sham molecular orbitals. Blue and red refer to positive and negative sign of the molecular orbitals. The orbital 1S is located inside the d band.

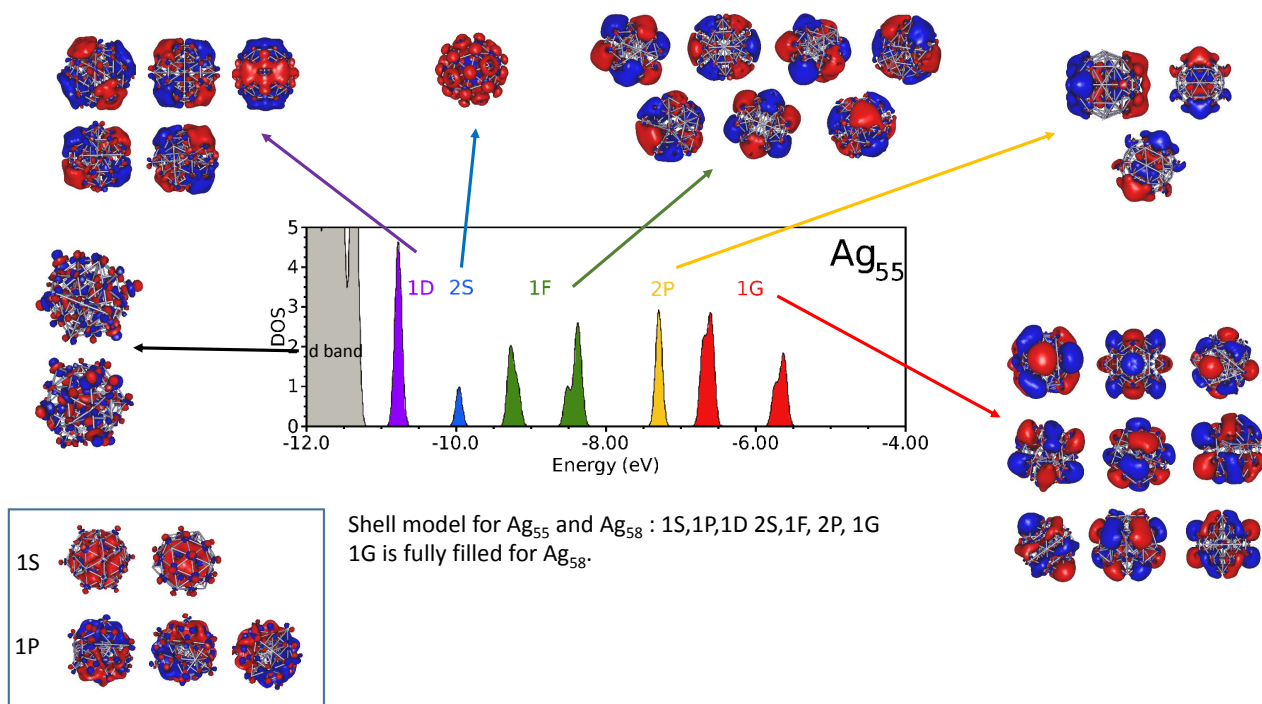


Figure S2: Density of states of Ag_{55} together with the representative Kohn-Sham molecular orbitals. Blue and red refer to positive and negative sign of the molecular orbitals. The orbitals 1S and 1P are located inside the d band.

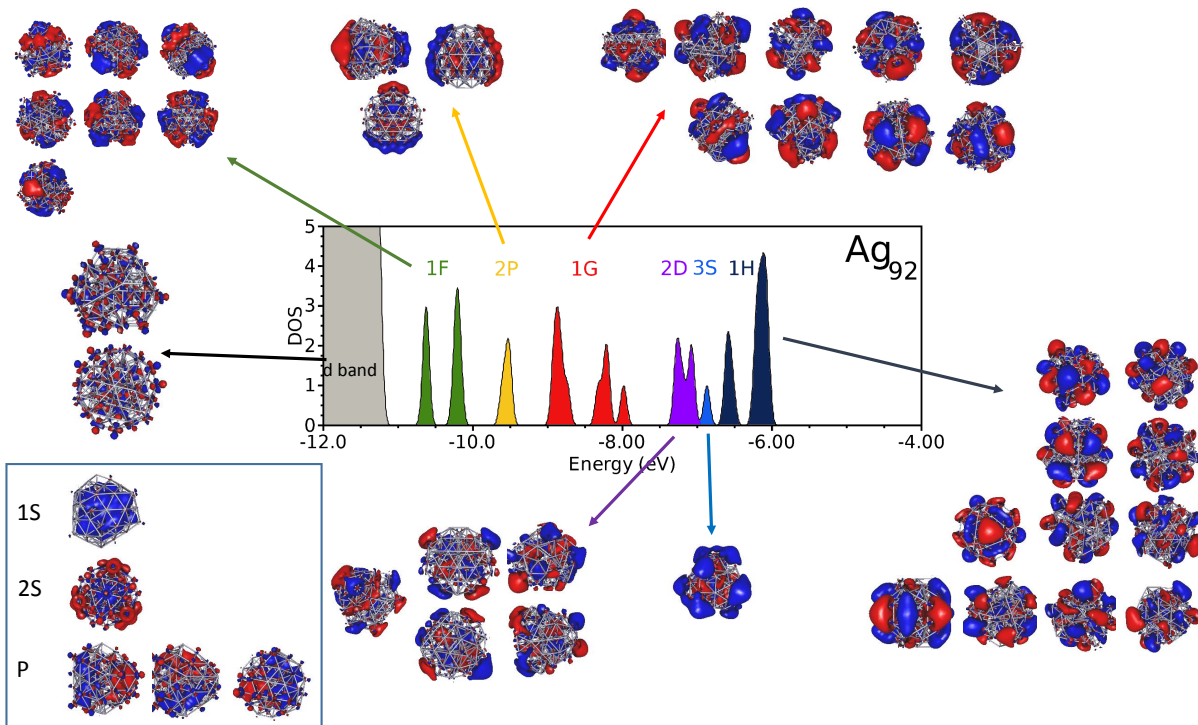


Figure S3: Density of states of Ag_{92} together with the representative Kohn-Sham molecular orbitals. Blue and red refer to positive and negative sign of the molecular orbitals. The orbitals 1S, 1P, 1D, and 2S are located inside the d band.

Notes and references

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- 5 M. Harb, F. Rabilloud, D. Simon, A. Rydlo, S. Lecoultre, F. Conus, V. Rodrigues and C. Félix, *J. Chem. Phys.*, 2008, **129**, 194108.
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Optimized coordinates of Ag_n@Ne₁₀₀.

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Ne	-3.0097200000	-11.9451150000	6.0670530000
Ne	-3.8933520000	7.4974450000	7.7928160000
Ne	-8.1965530000	2.0469790000	8.1822110000
Ne	8.4037530000	1.4938300000	2.7735080000
Ne	3.6813980000	13.3971090000	3.5316780000
Ne	0.1826930000	-5.8488260000	10.9127670000
Ne	-8.8844210000	7.8498280000	4.8620440000

Ag92Ne100

Ag	-4.3189520000	-3.9416540000	2.4157670000
Ag	-5.7986000000	-1.2695260000	2.4240730000
Ag	-4.4304990000	-0.4934820000	0.0000000000
Ag	-1.6313000000	-0.7039450000	0.0000000000
Ag	-4.5161830000	1.2898620000	2.5822190000
Ag	-4.2090810000	4.0065550000	1.5376140000
Ag	-2.4918790000	5.9043280000	0.0000000000
Ag	1.0647620000	2.3691460000	-2.3800130000
Ag	-1.3379760000	3.8188750000	-1.5001640000
Ag	-2.4147590000	5.8838190000	-2.9816770000
Ag	2.3893950000	2.9858010000	-4.7806460000
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Ag	-2.9452040000	0.4487220000	-4.8873310000
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Ag	-2.9677660000	-1.3797680000	-2.3517890000
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Ag	-7.1523790000	-0.3672550000	0.0000000000
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Ag	2.9528140000	-4.7659320000	-4.3473370000
Ag	1.8662560000	-2.6477260000	-2.8633920000
Ag	-0.6418850000	-2.9559920000	-1.5272230000
Ag	-1.9610190000	-3.8873820000	-3.9824190000
Ag	0.5082130000	-5.3975850000	0.0000000000
Ag	0.5371230000	-3.4324060000	-5.2496150000
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Ag	4.9872640000	-0.1203170000	3.8396370000
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Ag	2.1205750000	0.2067910000	3.8113980000
Ag	0.7956520000	-0.4422370000	-1.4147740000
Ag	0.7956520000	-0.4422370000	1.4147740000
Ag	-0.3437890000	1.7474890000	-5.0384970000
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Ag	0.1857700000	6.1857010000	1.5696170000
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Ag	-1.9901120000	-5.5021330000	1.4620940000
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Ne	-2.1097790000	0.6105170000	-8.4892350000
Ne	2.3845710000	-3.8814580000	-10.3056820000
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Ne	5.6603500000	-6.7633450000	-3.9382650000
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Ne	7.3894100000	5.0915010000	-8.0371080000
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Ne	6.7598500000	-1.2711470000	6.5496010000
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