Supporting Information

On the nature of Noble gas – Metal bond in Silver aggregates

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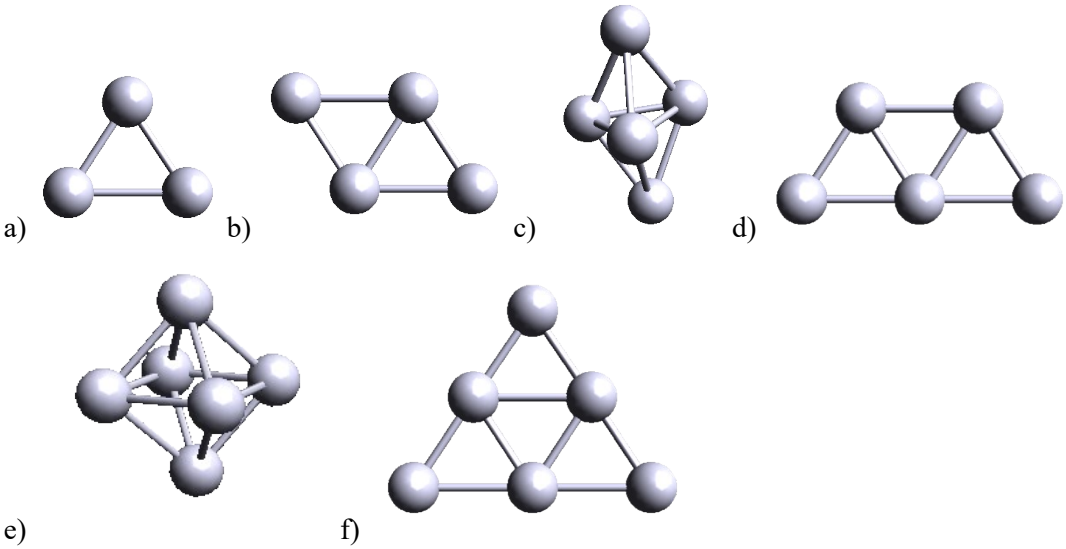

Figure S1 : Structures of the Ag_n aggregates: *a) Ag_3 b) Ag_4 c) Ag_5 3D, d) Ag_5 2D, e) Ag_6 3D f) Ag_6 2D*

Table S1 : Atoms-in-Molecules BCP descriptors of Ag_{147}

Ag147	Laplacian	Density at BCP	Gb(rc)	Vb(rc)	Hb(rc)	R	Theta
Xe Vertex	3,61E-02	1,62E-02	9,01E-03	-8,99E-03	2,14E-05	4,52E-03	8,97E+01
Xe Edge	1,50E-02	6,81E-03	3,20E-03	-2,65E-03	5,45E-04	1,95E-03	7,38E+01
Xe FCC	4,98E-03	2,64E-03	9,75E-04	-7,04E-04	2,71E-04	6,79E-04	6,65E+01
Xe HCP	5,51E-03	2,66E-03	1,07E-03	-7,52E-04	3,13E-04	7,57E-04	6,56E+01
Xe Facet	1,12E-02	5,21E-03	2,32E-03	-1,83E-03	4,86E-04	1,49E-03	7,09E+01

Table S2 : Atoms-in-Molecules BCP descriptors of Ag_{55}

Ag55	Laplacian	Density at BCP	Gb(rc)	Vb(rc)	Hb(rc)	R	Theta
He Vertex	8,02E-03	2,18E-03	1,44E-03	-8,79E-04	5,63E-04	0,00115	60,67736
He Edge	6,66E-03	1,83E-03	1,19E-03	-7,12E-04	4,76E-04	9,59E-04	60,22016
He FCC	4,02E-03	1,34E-03	7,17E-04	-4,29E-04	2,88E-04	5,79E-04	60,16123
He HCP	3,59E-03	1,22E-03	6,38E-04	-3,79E-04	2,59E-04	5,18E-04	59,99176
Ne Vertex	1,47E-02	3,94E-03	2,73E-03	-1,79E-03	9,43E-04	0,00207	62,83825
Ne Edge	1,15E-02	3,19E-03	2,12E-03	-1,36E-03	7,60E-04	0,00163	62,1394
Ne FCC	4,70E-03	1,65E-03	8,49E-04	-5,24E-04	3,26E-04	6,72E-04	61,01057
Ne HCP	6,50E-03	2,29E-03	1,20E-03	-7,70E-04	4,27E-04	9,18E-04	62,25243
Ar Vertex	1,46E-02	5,01E-03	2,85E-03	-2,06E-03	7,95E-04	0,00199	66,44835
Ar Edge	9,79E-03	3,36E-03	1,85E-03	-1,25E-03	5,99E-04	0,00136	63,90367
Ar FCC	4,03E-03	1,73E-03	7,43E-04	-4,79E-04	2,64E-04	5,69E-04	62,32004
Ar HCP	4,29E-03	1,85E-03	7,95E-04	-5,18E-04	2,77E-04	6,04E-04	62,64334
Kr Vertex	3,03E-02	1,11E-02	6,64E-03	-5,70E-03	9,39E-04	0,0039	76,07439
Kr Edge	2,52E-02	9,25E-03	5,37E-03	-4,44E-03	9,30E-04	0,00328	73,55675
Kr FCC	6,20E-03	2,92E-03	1,20E-03	-8,59E-04	3,45E-04	8,48E-04	65,97937
Kr HCP	4,20E-03	1,98E-03	7,90E-04	-5,29E-04	2,60E-04	5,86E-04	63,62225
Xe Vertex	4,22E-02	1,89E-02	1,09E-02	-1,12E-02	-3,34E-04	0,00529	93,62002
Xe Edge	2,31E-02	9,95E-03	5,17E-03	-4,57E-03	6,03E-04	0,00295	78,19718
Xe FCC	2,18E-02	6,70E-03	4,32E-03	-3,18E-03	1,13E-03	0,00295	67,42388
Xe HCP	5,11E-03	2,66E-03	9,98E-04	-7,19E-04	2,79E-04	6,97E-04	66,38897
Rn Vertex	4,40E-02	2,28E-02	1,26E-02	-1,42E-02	-1,60E-03	0,00573	106,19195
Rn Edge	3,26E-02	1,58E-02	8,29E-03	-8,43E-03	-1,40E-04	0,00408	91,96498
Rn FCC	9,82E-03	5,49E-03	2,13E-03	-1,80E-03	3,28E-04	0,00127	75,0298
Rn HCP	1,06E-02	5,72E-03	2,29E-03	-1,93E-03	3,58E-04	0,00137	74,87842

Table S3 : Atoms-in-Molecules BCP descriptors of Ag_{13}

Ag13	Laplacian	Density at BCP	Gb(rc)	Vb(rc)	Hb(rc)	R	Theta
He Hollow	3,14E-03	1,12E-03	5,58E-04	-3,31E-04	2,27E-04	4,53E-04	59,95895
He On-Top	5,78E-03	1,65E-03	1,03E-03	-6,14E-04	4,16E-04	8,33E-04	60,09649
Ne Hollow	5,83E-03	2,17E-03	1,08E-03	-6,95E-04	3,81E-04	8,23E-04	62,37409
Ne On-Top	1,38E-02	3,80E-03	2,57E-03	-1,68E-03	8,84E-04	0,00194	62,85834
Ar Hollow	6,58E-03	2,96E-03	1,27E-03	-8,99E-04	3,73E-04	9,03E-04	65,5987
Ar On-Top	2,45E-02	8,08E-03	5,02E-03	-3,91E-03	1,11E-03	0,00326	70,11823
Kr Hollow	2,50E-03	1,23E-03	4,57E-04	-2,89E-04	1,68E-04	3,55E-04	61,76728
Kr On-Top	3,48E-02	1,28E-02	7,81E-03	-6,92E-03	8,89E-04	0,00444	78,45002
Xe Hollow	3,92E-03	2,20E-03	7,60E-04	-5,40E-04	2,20E-04	5,37E-04	65,8387
Xe On-Top	5,71E-02	2,57E-02	1,59E-02	-1,76E-02	-1,67E-03	0,00733	103,153
Rn Hollow	1,28E-02	6,97E-03	2,86E-03	-2,53E-03	3,36E-04	0,00163	78,12507
Rn On-Top	5,67E-02	2,85E-02	1,71E-02	-2,00E-02	-2,91E-03	0,00766	112,32229

Table S4 : Atoms-in-Molecules BCP descriptors of Ag_1

Ag1	Laplacian	Density at BCP	Gb(rc)	Vb(rc)	Hb(rc)	R	Theta
He	3,53E-03	1,13E-03	6,24E-04	-3,65E-04	2,59E-04	5,12E-04	59,59153
Ne							
Ar	1,16E-02	4,47E-03	2,28E-03	-1,66E-03	6,18E-04	0,00158	66,90266
Kr	1,32E-02	5,85E-03	2,75E-03	-2,19E-03	5,55E-04	0,00174	71,41932
Xe	2,49E-02	1,20E-02	5,96E-03	-5,69E-03	2,69E-04	0,00312	85,0594
Rn	3,34E-02	1,84E-02	9,25E-03	-1,02E-02	-8,99E-04	0,00427	102,14916

Table S5 : Atoms-in-Molecules BCP descriptors of Ag_2

Ag2	Laplacian	Density at BCP	Gb(rc)	Vb(rc)	Hb(rc)	R	Theta
He	0,00809	0,00218	0,00145	-8,85E-04	5,69E-04	0,00116	60,63782
Ne	0,0166	0,00428	0,00309	-0,00203	0,00106	0,00233	62,95354
Ar	0,0371	0,0116	0,00789	-0,00651	0,00138	0,00484	73,37236
Kr	0,0507	0,0186	0,0122	-0,01172	4,76E-04	0,00636	85,70529
Xe	0,0694	0,0308	0,02026	-0,02316	-0,00291	0,00915	108,52011
Rn	0,0545	0,0284	0,01667	-0,01972	-0,00305	0,00746	114,10964

Table S6 : Atoms-in-Molecules BCP descriptors of Ag_3

Ag3	Laplacian	Density at BCP	Gb(rc)	Vb(rc)	Hb(rc)	R	Theta
He	6,73E-03	1,76E-03	1,20E-03	-7,08E-04	4,87E-04	9,72E-04	59,9248
Ne	1,28E-02	3,47E-03	2,36E-03	-1,52E-03	8,38E-04	0,00181	62,34805
Ar	4,59E-02	1,42E-02	1,00E-02	-8,61E-03	1,43E-03	0,00591	75,96571
Kr	7,90E-02	2,79E-02	2,05E-02	-2,13E-02	-7,86E-04	0,00991	94,54897
Xe	7,78E-02	3,51E-02	2,38E-02	-2,81E-02	-4,32E-03	0,01064	113,95433
Rn	6,62E-02	3,42E-02	2,14E-02	-2,62E-02	-4,83E-03	0,00958	120,26883

Table S7: Atoms-in-Molecules BCP descriptors of Ag_4

Ag4	Laplacian	Density at BCP	Gb(rc)	Vb(rc)	Hb(rc)	R	Theta
He	0,0249	0,00582	0,00469	-0,00316	0,00153	0,00347	63,75881
Ne	0,0358	0,00775	0,00684	-0,00473	0,00211	0,00495	64,73591
Ar	0,0717	0,0214	0,01669	-0,01545	0,00124	0,00905	82,13007
Kr	0,101	0,034	0,02708	-0,02891	-0,00183	0,01276	98,24245
Xe	0,0869	0,0373	0,02644	-0,03115	-0,00471	0,01184	113,46056
Rn	0,0841	0,0408	0,0279	-0,03478	-0,00688	0,01256	123,18505

Table S8: Atoms-in-Molecules BCP descriptors of Ag_6 Octahedron

Ag6	Laplacian	Density at BCP	Gb(rc)	Vb(rc)	Hb(rc)	R	Theta
He	4,69E-03	1,40E-03	8,32E-04	-4,91E-04	3,41E-04	6,78E-04	59,83483
Ne	2,11E-02	7,36E-03	4,32E-03	-3,36E-03	9,57E-04	0,0028	70,04466
Ar	3,89E-02	1,48E-02	9,03E-03	-8,34E-03	6,85E-04	0,0049	81,97588
Kr	5,63E-02	2,61E-02	1,60E-02	-1,79E-02	-1,92E-03	0,00729	105,25263
Xe	5,04E-02	2,32E-02	1,38E-02	-1,51E-02	-1,23E-03	0,00642	101,0057
Rn	5,03E-02	2,32E-02	1,38E-02	-1,50E-02	-1,22E-03	0,00641	100,98822

Table S9 : Values of R_0 of the power law fit for each noble gas

Gas	R0	R-square
He	1,4382	0,948
Ne	1,5272	0,920
Ar	1,7003	0,979
Kr	1,7581	0,960
Xe	1,8368	0,971
Rn	1,8536	0,943

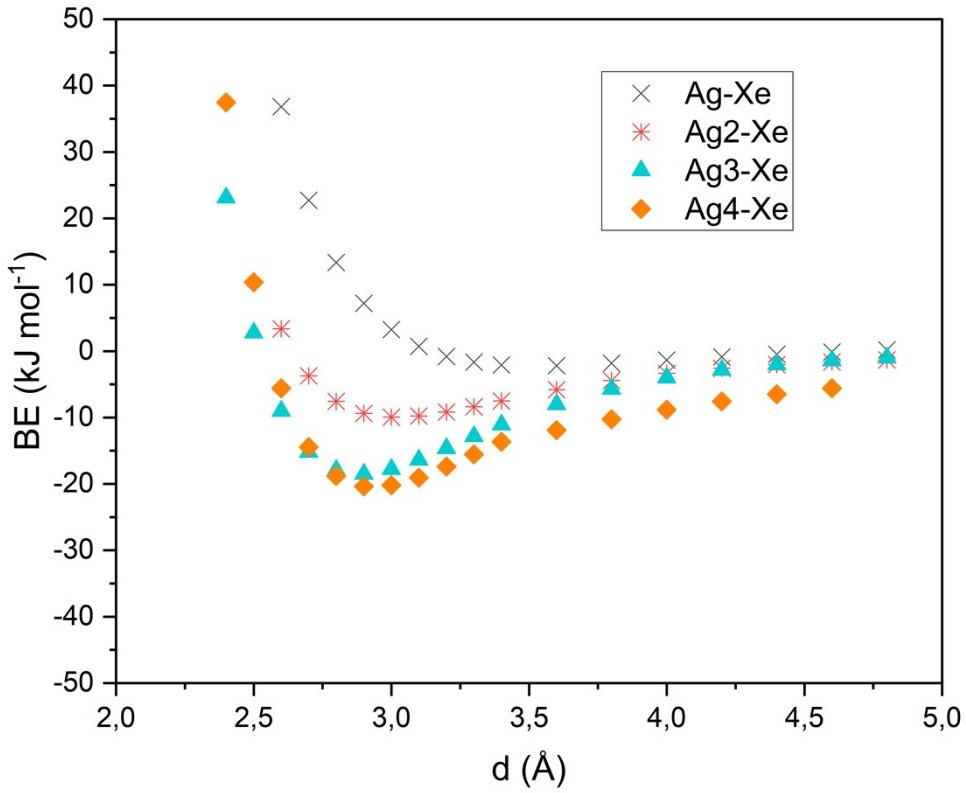

Figure S2: Binding energy curves of Xe to Ag_1, Ag_2, Ag_3 and Ag_4

Table S10: Binding energies and bond lengths of Xe with Ag_1, Ag_2, Ag_3 and Ag_4

System size (Ag_n)	**Binding Energy (kJ mol^{-1})**	**Bond length (Å)**
Ag_1	-2.18	3.6
Ag_2	-9,96	3.0
Ag_3	-18.49	2.9
Ag_4	-20.37	2.9

Table S11: Relative energies and bond length of Ag_{55}-Xe for each inequivalent adsorption site.

Adsorption site	**Relative energy (kJ mol^{-1})**	**Bond length (Å)**
Vertex S5	0 *(reference)*	3.3
Edge S6	+3.16	3.6
Hollow FCC	+6.98	3.6
Hollow HCP	+4.18	4.1