Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Structural evolution of $(Au_2S)_n$ (n = 1–8) clusters from first principles global optimization

By

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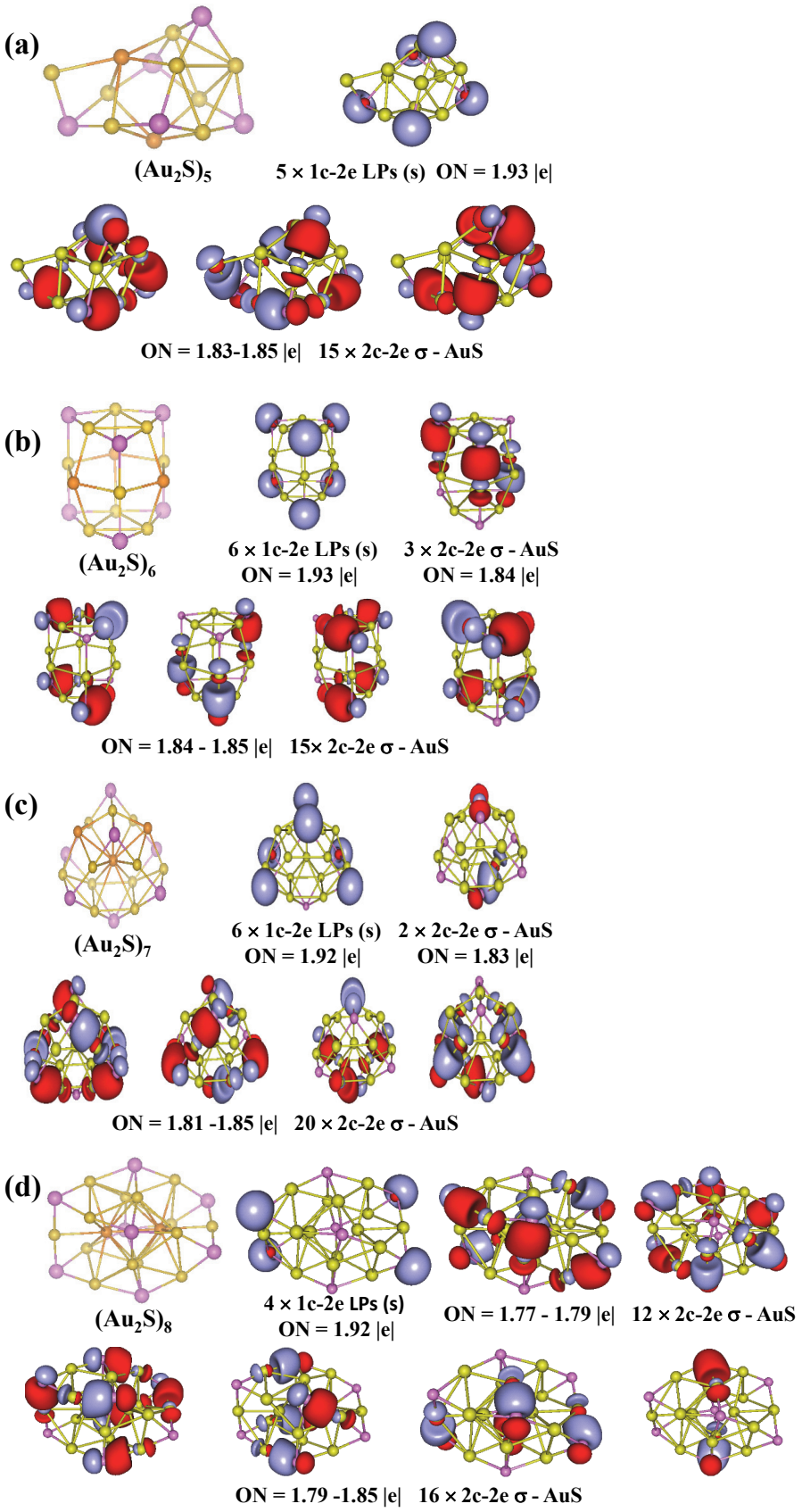

Figure S1. AdNDP localized chemical bonding orbitals of the global minimum structures of $(Au_2S)_n$ (n = 5-8) at TPSS/Lanl2DZ/6-31G* level of theory. ON gives the occupancy numbers.

The atomic coordinates (in Å) of the global minimum structures of $(Au_2S)_n$ (n = 1-8) clusters.

1A：	Au	0.000000	1.620713	-0.147210
	Au	0.000000	-1.620713	-0.147210
	S	0.000000	0.000000	1.453700
2A：	Au	-0.171453	1.349461	-0.154460
	Au	0.171453	-1.349461	-0.154460
	Au	-2.496302	-0.823644	0.206879
	Au	2.496302	0.823644	0.206879
	S	-2.496302	1.437622	-0.258821
	S	2.496302	-1.437622	-0.258821
3A：	Au	0.359687	-0.858867	1.508377
	Au	0.359687	-0.858867	-1.508377
	Au	-1.938135	1.232629	2.294601
	Au	2.641667	-2.510111	0.000000
	Au	0.299097	1.754181	0.000000
	Au	-1.938135	1.232629	-2.294601
	S	0.347777	-2.753979	0.000000
	S	0.359687	1.397741	2.388983
	S	0.359687	1.397741	-2.388983
4A:	Au	1.552327	1.832801	0.601278
	Au	-1.552327	1.832801	0.601278
	Au	0.000000	2.322672	-2.305451
	Au	0.000000	0.000000	2.391517
	Au	-1.552327	-1.832801	0.601278
	Au	0.000000	0.000000	-0.833112
	Au	1.552327	-1.832801	0.601278
	Au	0.000000	-2.322672	-2.305451
	S	0.000000	3.504745	-0.302467
	S	-2.432609	0.000000	1.900698
	S	2.432609	0.000000	1.900698
	S	0.000000	-3.504745	-0.302467
5A：	Au	1.401126	-0.056963	2.518421
	Au	1.659414	2.364174	0.000000
	Au	-0.973570	2.103308	1.541170
	Au	0.208921	0.036736	0.000000
	Au	1.512223	-2.447920	0.000000
	Au	-2.733154	-0.496410	0.000000
	Au	-0.980435	-1.941926	1.579001

	Au	1.401126	-0.056963	-2.518421
	Au	-0.973570	2.103308	-1.541170
	Au	-0.980435	-1.941926	-1.579001
	S	1.268129	-2.453449	2.407473
	S	1.281303	2.331786	2.412889
	S	-2.835738	1.895326	0.000000
	S	1.268129	-2.453449	-2.407473
	S	1.281303	2.331786	-2.412889
6A：	Au	0.000000	2.430405	1.206868
	Au	-2.492494	-1.485702	0.656439
	Au	-2.492494	1.485702	0.656439
	Au	0.000000	0.000000	2.627257
	Au	-2.347393	0.000000	-1.955182
	Au	0.000000	-2.430405	1.206868
	Au	2.492494	-1.485702	0.656439
	Au	0.000000	-2.478209	-1.608549
	Au	2.492494	1.485702	0.656439
	Au	0.000000	2.478209	-1.608549
	Au	0.000000	0.000000	-0.295504
	Au	2.347393	0.000000	-1.955182
	S	-2.420479	0.000000	2.598939
	S	-2.402520	2.409511	-1.600391
	S	-2.402520	-2.409511	-1.600391
	S	2.420479	0.000000	2.598939
	S	2.402520	-2.409511	-1.600391
	S	2.402520	2.409511	-1.600391
7A：	Au	0.000000	3.602576	-0.690586
	Au	0.000000	0.000000	-0.026023
	Au	1.480864	-1.438932	-2.140399
	Au	2.433846	1.585597	0.951607
	Au	1.480864	1.438932	-2.140399
	Au	-2.433846	1.585597	0.951607
	Au	-1.480864	1.438932	-2.140399
	Au	-1.480864	-1.438932	-2.140399
	Au	0.000000	2.491896	1.764068
	Au	2.433846	-1.585597	0.951607
	Au	0.000000	-2.491896	1.764068
	Au	0.000000	-3.602576	-0.690586
	Au	-2.433846	-1.585597	0.951607
	Au	0.000000	0.000000	2.886890
	S	-2.407675	3.226731	-0.805230
	S	0.000000	0.000000	-3.572480

	S	2.407675	3.226731	-0.805230
	S	2.417206	0.000000	2.772941
	S	2.407675	-3.226731	-0.805230
	S	-2.407675	-3.226731	-0.805230
	S	-2.417206	0.000000	2.772941
8A：	Au	0.000000	0.000000	4.234242
	Au	-1.225237	2.419393	2.414415
	Au	0.000000	0.000000	1.443225
	Au	1.792796	2.088981	2.189262
	Au	-2.516618	0.000000	0.218089
	Au	0.000000	2.516618	-0.218089
	Au	-1.792796	-2.088981	2.189262
	Au	1.225237	-2.419393	2.414415
	Au	-2.088981	1.792796	-2.189262
	Au	-2.419393	-1.225237	-2.414415
	Au	2.516618	0.000000	0.218089
	Au	2.088981	-1.792796	-2.189262
	Au	0.000000	0.000000	-1.443225
	Au	0.000000	-2.516618	-0.218089
	Au	2.419393	1.225237	-2.414415
	Au	0.000000	0.000000	-4.234242
	S	0.433829	2.346822	4.169612
	S	-2.485084	2.457617	0.268913
	S	-0.433829	-2.346822	4.169612
	S	-2.457617	-2.485084	-0.268913
	S	2.485084	-2.457617	0.268913
	S	2.457617	2.485084	-0.268913
	S	-2.346822	0.433829	-4.169612
	S	2.346822	-0.433829	-4.169612