

## **Supplementary materials**

### **Study of the geometric structures, electronic and magnetic properties of aluminum-antimony alloy clusters**

Ai-Jie Mao<sup>\*</sup>, Xiao-Yu Kuang, Hao Cheng, Li-Huan Zhang, Xiao-Rong Cheng

Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China

<sup>\*</sup>Correspondence

author. E-mail: scu\_mij@126.com

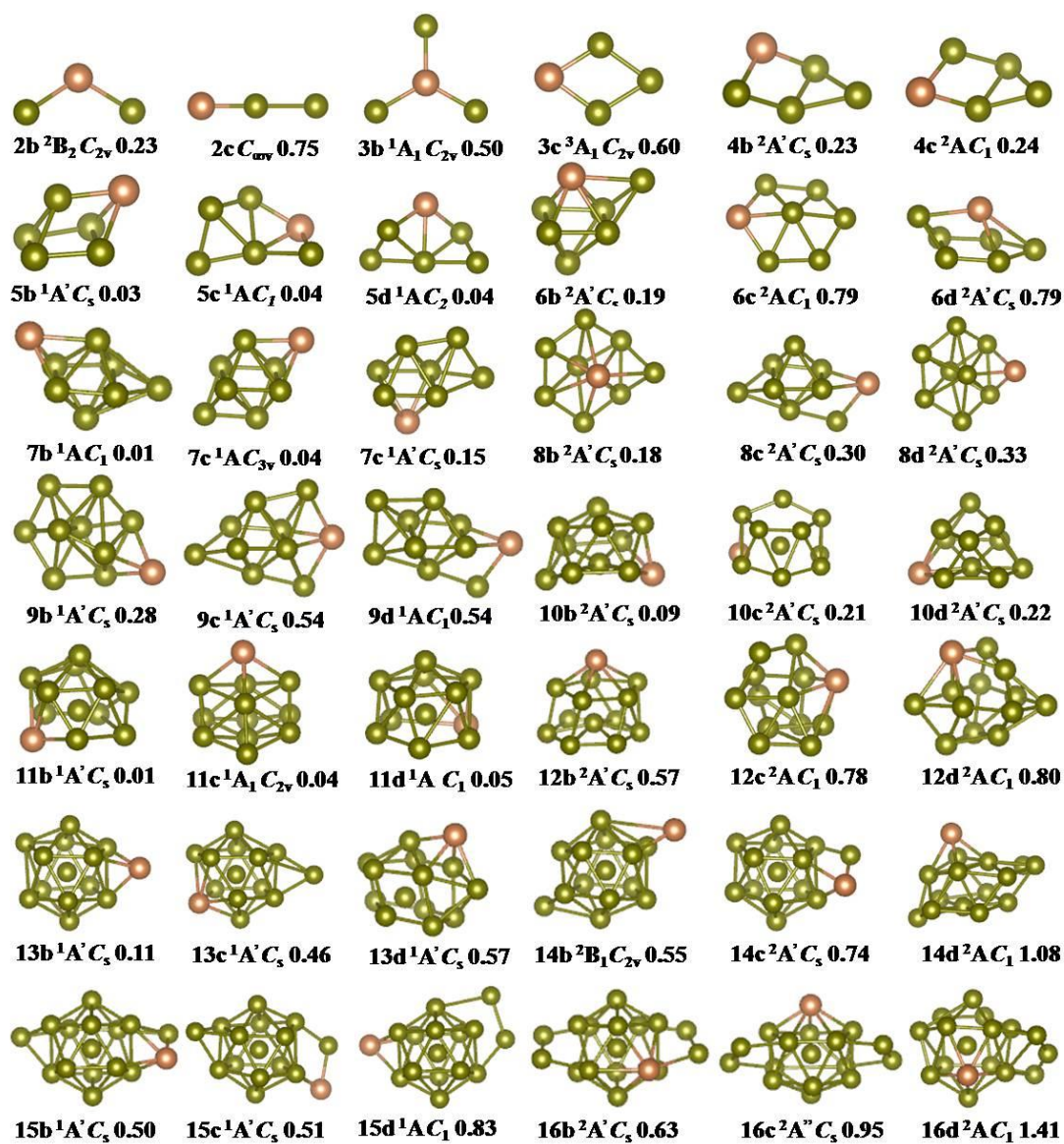
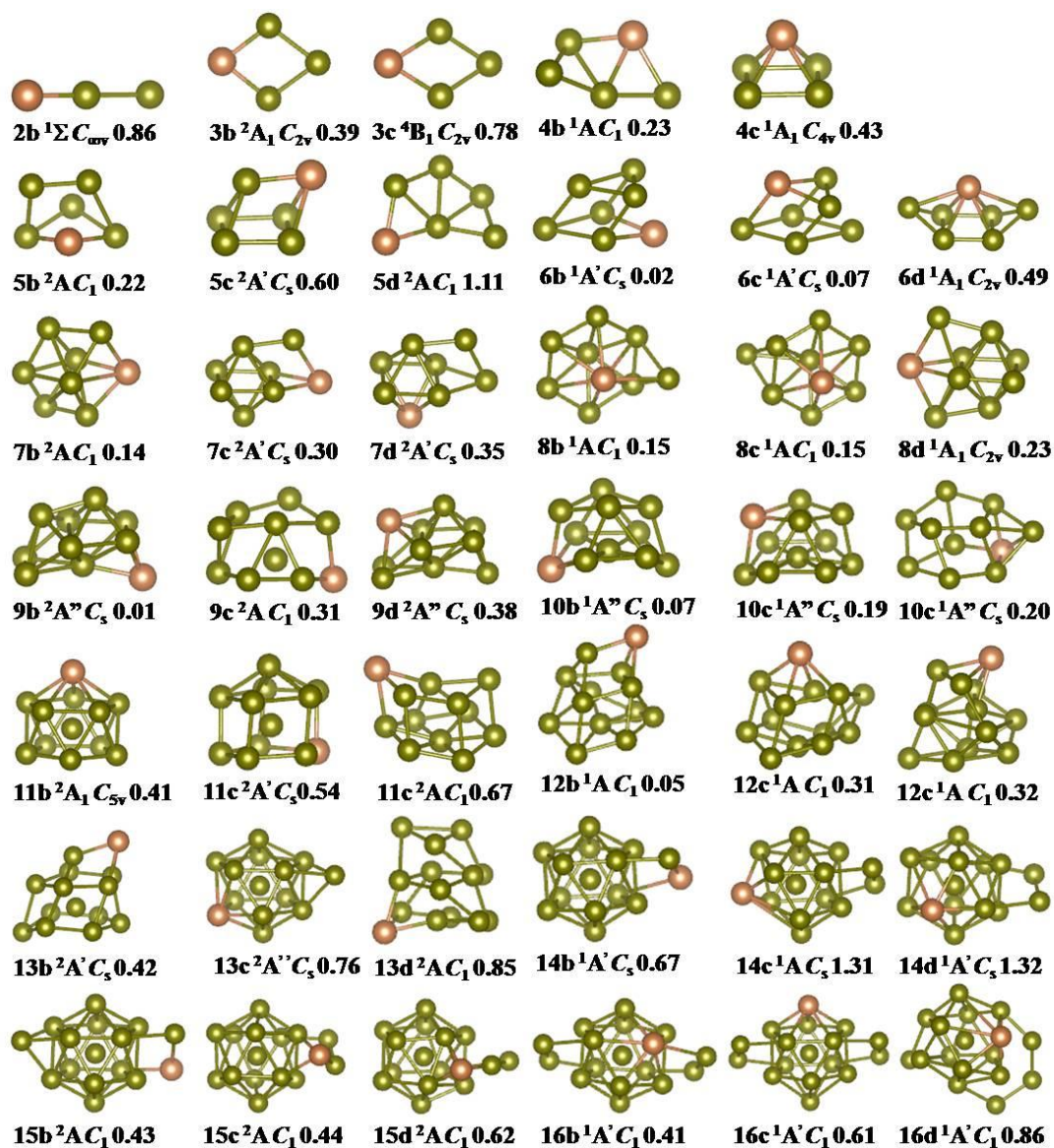
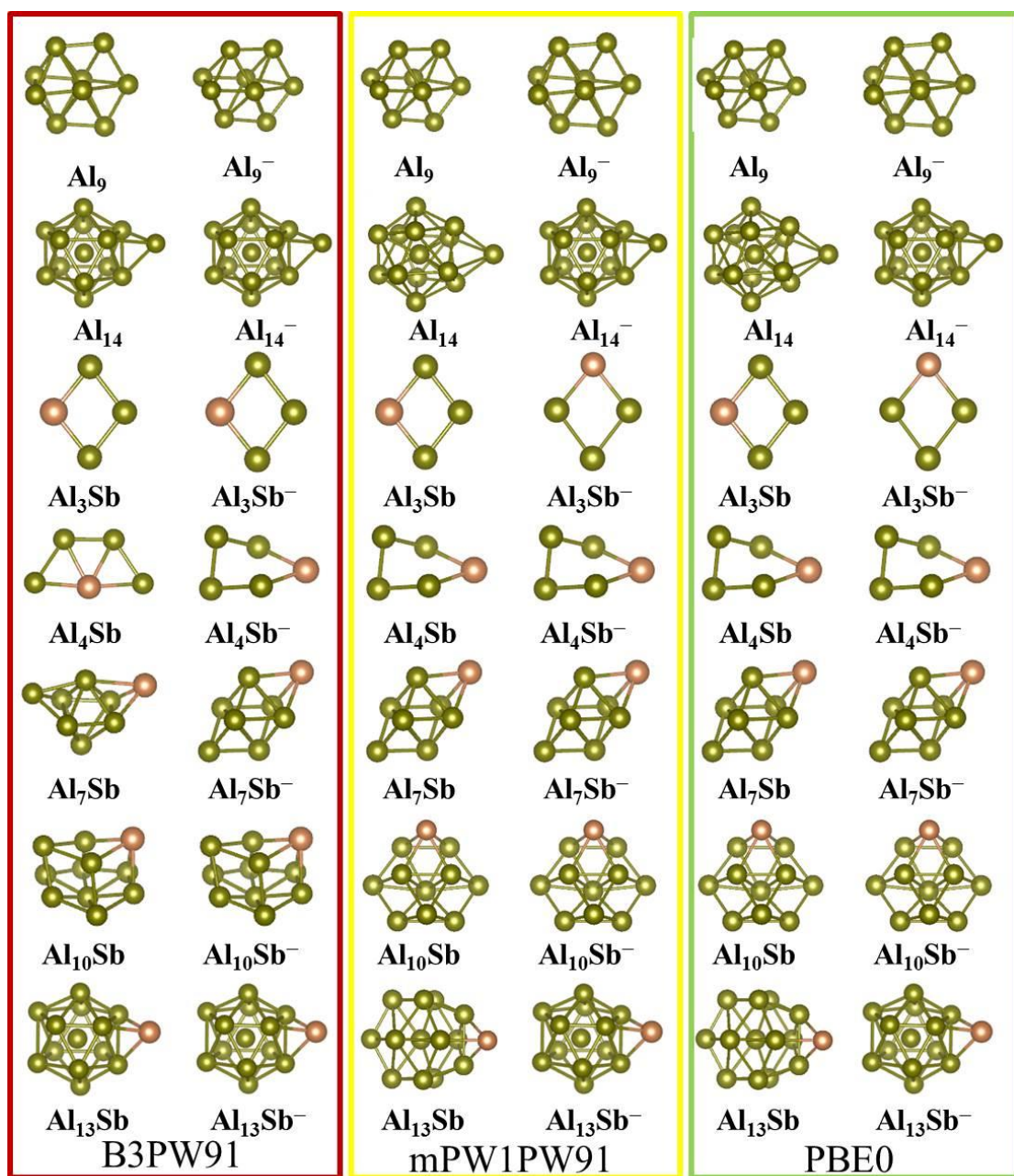


Fig. S1 The metastable isomers of  $Al_nSb$  ( $n=1-16$ ) clusters, together with point symmetry and relative energies.



**Fig. S2** The metastable isomers of  $Al_nSb^-$  ( $n=1-16$ ) clusters, together with point symmetry and relative energies.



**Fig. S3** The clusters possess different ground state structure for neutral and anion  $\text{Al}_{n+1}$  and  $\text{Al}_n\text{Sb}$  ( $n=1-16$ ) clusters based on different functionals.



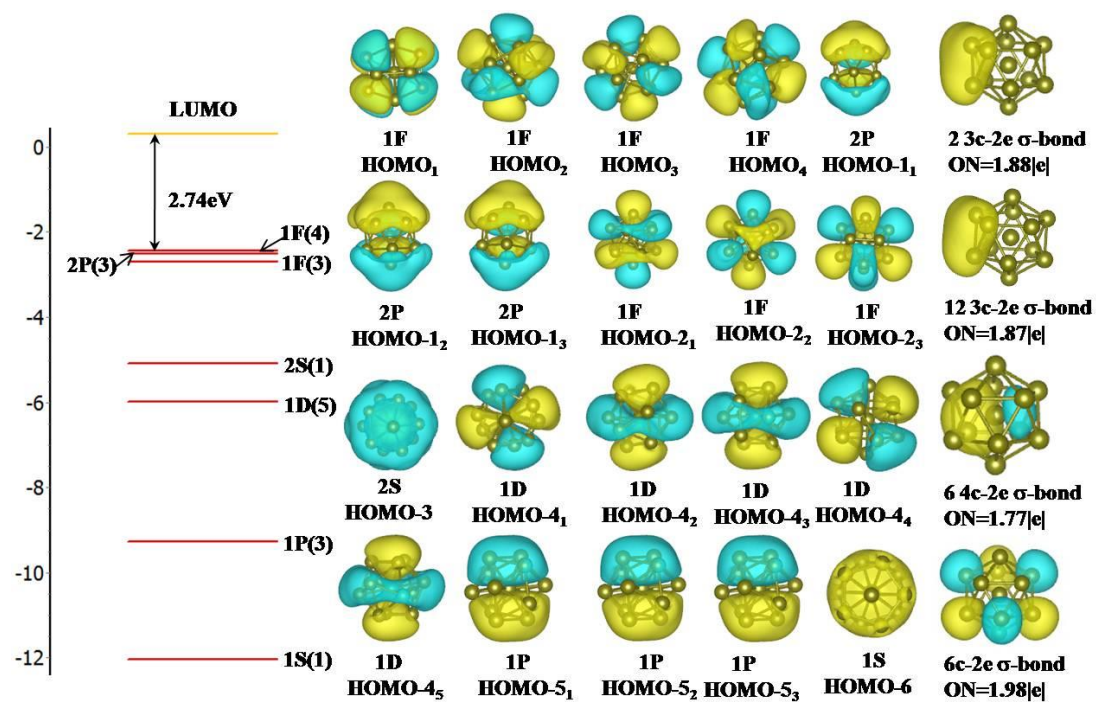


Fig. S4 Calculated molecular orbital energy levels and AdNDP chemical bonding analysis of the most stable structure of  $\text{Al}_{13}^-$  clusters together with the molecular orbital maps of the HOMOs. where, ON presents for occupation number.

Table S1. Electronic states, symmetries, average binding energies  $E_b$  (eV) and HOMO–LUMO energy gaps  $E_{\text{gap}}$  (eV) of the most stable structures for  $\text{Al}_{n+1}^q$  ( $q=0,-1$ ,  $n=1-16$ ) clusters.

clusters	State	Symm	$E_b$	$E_{\text{gap}}$	$\eta$	clusters	State	Symm	$E_b$	$E_{\text{gap}}$
$\text{Al}_2$		$D_{\infty h}$	0.72	1.31	3.60	$\text{Al}_2^-$	$^4\Sigma_g$	$D_{\infty h}$	1.25	2.06
$\text{Al}_3$	$^2\text{A}_1'$	$D_{3h}$	1.20	1.63	2.55	$\text{Al}_3^-$	$^1\text{A}_1$	$D_{3h}$	1.62	1.57
$\text{Al}_4$	$^1\text{A}_g$	$C_{2h}$	1.35	1.15	2.14	$\text{Al}_4^-$	$^2\text{A}_g$	$C_{2h}$	1.83	1.53
$\text{Al}_5$	$^2\text{B}_2$	$C_{2v}$	1.62	1.78	2.35	$\text{Al}_5^-$	$^1\text{A}'$	$C_s$	1.95	1.36
$\text{Al}_6$	$^1\text{A}_{1g}$	$D_{3d}$	1.81	1.64	2.29	$\text{Al}_6^-$	$^2\text{A}_{1g}$	$D_{3d}$	2.15	2.19
$\text{Al}_7$	$^2\text{A}_1$	$C_{3v}$	2.03	1.80	2.27	$\text{Al}_7^-$	$^1\text{A}_1$	$C_{3v}$	2.27	1.61
$\text{Al}_8$	$^1\text{A}_g$	$C_{2h}$	2.06	1.86	2.29	$\text{Al}_8^-$	$^2\text{A}'$	$C_s$	2.28	1.51
$\text{Al}_9$	$^2\text{A}'$	$C_s$	2.11	0.86	2.24	$\text{Al}_9^-$	$^1\text{A}$	$C_2$	2.35	1.49
$\text{Al}_{10}$	$^1\text{A}'$	$C_s$	2.17	1.53	2.05	$\text{Al}_{10}^-$	$^2\text{A}'$	$C_s$	2.38	1.50
$\text{Al}_{11}$	$^2\text{A}_1$	$C_{2v}$	2.22	1.78	1.91	$\text{Al}_{11}^-$	$^1\text{A}'$	$C_s$	2.42	1.54
$\text{Al}_{12}$	$^1\text{A}_1$	$C_{2v}$	2.83	1.99	2.24	$\text{Al}_{12}^-$	$^2\text{A}'$	$C_s$	2.45	1.19
$\text{Al}_{13}$	$^1\text{A}$	$D_{3d}$	2.37	1.32	1.88	$\text{Al}_{13}^-$	$^1\text{A}$	$I_h$	2.59	2.74
$\text{Al}_{14}$	$^2\text{A}_1$	$C_3$	2.40	1.75	2.02	$\text{Al}_{14}^-$	$^2\text{B}_2$	$C_{2v}$	2.55	1.34
$\text{Al}_{15}$	$^2\text{B}_{3u}$	$D_{2h}$	2.41	1.49	1.85	$\text{Al}_{15}^-$	$^1\text{A}$	$D_{3d}$	2.56	1.51
$\text{Al}_{16}$	$^1\text{A}'$	$C_s$	2.43	1.60	1.90	$\text{Al}_{16}^-$	$^2\text{A}'$	$C_s$	2.57	1.48
$\text{Al}_{17}$	$^2\text{B}_{2u}$	$D_{2h}$	2.45	1.43	1.68	$\text{Al}_{17}^-$	$^1\text{A}_g$	$D_{2h}$	2.58	1.41

Table S2. The calculated *ADE* and *VDE* values of the most stable structures for  $\text{Al}_n\text{Sb}$  ( $n=1-16$ ) clusters based on different functionals, together with available experimental data.

	ADE				VDE			
	mPW1PW91	PBE0	B3PW91	Expt. <sup>1</sup>	mPW1PW91	PBE0	B3PW91	Expt. <sup>1</sup>
1	1.92	1.96	1.99	1.89	2.01	2.04	2.03	2.13
2	2.28	2.25	2.31	2.34	2.49	2.48	2.50	2.57
3	1.64	1.62	2.00	1.88	2.31	2.31	2.67	2.27
4	2.36	2.35	2.16	1.96	2.50	2.50	2.51	2.62
5	2.35	2.35	2.32	2.21	2.78	2.77	2.75	2.87
6	2.24	2.22	2.27		2.57	2.54	2.63	
7	2.60	2.60	2.54		2.87	2.87	2.84	
8	2.47	2.47	2.49		2.64	2.63	2.66	
9	2.18	2.17	2.17		2.43	2.41	2.42	
10	2.65	2.65	2.66		2.75	2.74	2.76	
11	2.95	2.94	3.10		3.02	3.00	3.18	
12	2.42	2.40	2.44		2.80	2.77	2.81	
13	2.70	2.74	2.67		2.98	2.97	2.96	
14	2.80	2.80	2.82		3.12	3.12	3.14	
15	2.30	2.29	2.29		2.51	2.49	2.50	
16	2.63	2.61	2.64		2.83	2.80	2.83	

Table S3. The calculated *VIP* and *VEA* values of the most stable structures for  $\text{Al}_n\text{Sb}$  ( $n=1-16$ ) clusters based different functionals, together with available theoretical data.

Size	VEA				VIP			
	mPW1PW91	PBE0	B3PW91	Theor. <sup>1</sup>	mPW1PW91	PBE0	B3PW91	Theor. <sup>1</sup>
1	1.92	1.93	1.94	1.98	7.13	7.57	7.17	6.99
2	1.98	1.96	2.00	1.90	7.46	7.44	7.45	7.09
3	1.75	1.74	1.71	1.44	7.46	7.45	7.47	7.18
4	2.18	2.17	1.99	1.88	6.93	6.82	6.50	6.29
5	1.80	1.78	1.79	1.63	6.79	6.78	6.79	6.58
6	1.97	1.96	2.01	1.96	6.42	6.41	6.41	6.15
7	2.32	2.31	1.76		6.56	6.56	6.59	
8	2.32	2.32	2.34		6.49	6.49	6.46	
9	1.99	1.99	1.98		6.57	6.57	6.57	
10	2.54	2.55	2.55		6.28	6.28	6.26	
11	2.89	2.88	2.11		6.63	6.63	6.44	
12	2.06	2.05	2.08		6.18	6.17	6.16	
13	2.05	2.03	2.06		6.42	6.42	6.40	
14	2.48	2.48	2.51		6.26	6.26	6.24	
15	2.08	2.08	2.08		6.21	6.19	6.22	
16	2.40	2.39	2.41		5.83	5.80	5.81	

Table S4. The calculated *ADE* and *VDE* values of the most stable structures for  $\text{Al}_{n+1}^-$  ( $n=1-16$ ) clusters based on different functionals, together with available experimental and theoretical data.

Size	ADE				VDE				
	mPW1PW91	PBE0	B3PW91	Expt <sup>2,3</sup>	mPW1PW91	PBE0	B3PW91	Expt <sup>2,3</sup>	Theor <sup>4</sup>
1	1.60	1.60	1.54	1.20	1.62	1.62	1.62	1.61	1.45,1.47
2	1.73	1.72	1.75	1.40	1.73	1.72	1.75	1.92	1.52,1.53
3	2.43	2.42	2.41	1.80	2.54	2.53	2.53	2.20	2.38,2.39
4	2.11	2.11	2.13	1.92	2.16	2.15	2.19	2.13	1.97
5	3.81	2.56	2.52	2.31	2.81	2.81	2.79	2.63	2.63,2.62
6	2.10	2.10	2.11	2.08	2.40	2.39	2.41	2.49	2.13,2.14
7	2.15	2.28	2.26	2.11	2.34	2.54	2.45	2.45	2.03,2.05
8	2.84	2.83	2.63	2.57	3.04	3.02	3.05	2.91	2.67,2.68
9	2.65	2.65	2.62	2.42	2.86	2.86	2.83	2.94	2.49
10	2.73	2.71	2.70	2.51	2.80	2.78	2.80	2.92	
11	1.77	2.59	2.53	2.55	2.85	2.85	2.82	2.85	
12	3.41	3.42	3.40	3.42	3.66	3.65	3.66	3.68	
13	2.55	2.54	2.52	2.38	2.76	2.75	2.74	2.68	
14	2.79	2.78	2.77	2.39	2.98	2.97	2.96	3.02	
15	2.65	2.65	2.63	2.64	3.02	3.02	3.00	2.97	
16	2.69	2.68	2.72	2.78	2.87	2.86	2.89	2.98	



Table S5. The calculated *VIP* and *VEA* values of the most stable structures for  $\text{Al}_{n+1}$  (n=1-16) clusters based different functionals, together with available theoretical data.

Size	VEA				VIP			
	mPW1PW91	PBE0	B3PW91	Theor. <sup>4</sup>	mPW1PW91	PBE0	B3PW91	Theor. <sup>4</sup>
1	1.59	1.57	1.48		6.69	6.67	6.27	6.29
2	1.73	1.72	1.75	1.63	6.86	6.84	6.85	6.08,6.76,6.78
3	2.26	2.24	2.24	2.13	6.50	6.49	6.52	6.50,6.69,6.70
4	2.05	2.05	2.07	2.00	6.78	6.78	6.76	6.66,6.63,6.64
5	3.09	2.28	2.25	2.22	6.82	6.82	6.83	6.82,6.61
6	1.80	1.80	1.82	1.81	6.37	6.37	6.35	6.32,6.14,
7	1.98	1.97	1.97	1.96	6.56	6.55	6.55	6.48,6.24,6.25
8	2.66	2.65	2.45	2.36	6.70	6.69	6.93	6.57,6.37
9	2.39	2.39	2.36	2.29	6.46	6.45	6.47	6.32,5.96
10	2.60	2.58	2.51	2.52	6.32	6.30	6.34	6.30
11	1.91	1.91	1.91	2.12	7.16	6.36	6.39	6.29
12	3.13	3.14	3.11	3.10	6.90	6.93	6.87	6.84
13	2.32	2.32	2.29	2.22	6.16	6.15	6.34	6.31
14	2.58	2.57	2.29	2.53	6.17	6.16	6.00	6.09
15		2.21	2.24	2.21	6.04	6.03	6.04	6.02
16		2.50	2.54	2.51	5.90	5.89	5.89	5.86

Table S6. The average binding energies  $E_b$  (eV) of the most stable structures for  $Al_nSb^q$  and pure  $Al_{n+1}^q$  ( $q=0,-1, n=1-16$ ) clusters.

Size	$Al_nSb$			$Al_nSb$			$Al_{n+1}$				$Al_{n+1}$			
	mPW1PW91	PBE0	B3PW91	mPW1PW91	PBE0	B3PW91	mPW1PW91	PBE0	B3PW91	Theor. <sup>4</sup>	mPW1PW91	PBE0	B3PW91	Theor. <sup>4</sup>
1	0.77	0.79	0.79	1.42	1.56	1.54	0.69	0.71	0.72	0.76,0.75	1.23	1.27	1.25	1.37,1.35
2	1.35	1.38	1.35	1.73	1.99	1.96	1.21	1.24	1.20	1.27,1.24	1.63	1.66	1.62	1.73,1.69
3	1.73	1.76	1.73	1.72	2.06	2.10	1.36	1.39	1.35	1.48,1.44	1.84	1.88	1.83	1.95,1.91
4	1.74	1.78	1.77	1.79	2.17	2.10	1.65	1.69	1.62	1.70,1.66	1.97	2.01	1.95	2.07,2.02
5	1.99	2.05	1.98	1.96	2.37	2.28	1.62	1.88	1.81	1.91,1.86	2.18	2.23	2.15	2.30,2.25
6	2.07	2.12	2.04	1.94	2.38	2.29	2.07	2.13	2.03	2.15,2.09	2.30	2.35	2.27	2.41,2.35
7	2.13	2.18	2.09	2.00	2.45	2.35	2.09	2.15	2.06	2.16,2.10	2.30	2.37	2.28	2.40,2.34
8	2.23	2.28	2.19	2.05	2.51	2.41	2.13	2.19	2.11	2.13,2.17	2.39	2.45	2.35	2.49,2.43
9	2.29	2.35	2.25	2.05	2.52	2.41	2.21	2.27	2.17	2.27,2.21	2.42	2.48	2.38	2.52,2.46
10	2.30	2.36	2.25	2.08	2.56	2.45	2.26	2.32	2.22		2.47	2.53	2.42	
11	2.35	2.42	2.31	2.14	2.63	2.52	2.40	2.39	2.83		2.50	2.57	2.45	
12	2.44	2.52	2.39	2.17	2.67	2.54	2.42	2.49	2.37		2.65	2.72	2.59	
13	2.47	2.53	2.41	2.20	2.70	2.57	2.45	2.53	2.40		2.60	2.67	2.55	
14	2.52	2.59	2.46	2.24	2.75	2.61	2.46	2.53	2.41		2.61	2.69	2.56	
15	2.53	2.60	2.47	2.21	2.72	2.47	2.49	2.56	2.43		2.62	2.73	2.57	
16	2.49	2.56	2.44	2.18	2.69	2.56	2.51	2.57	2.45		2.64	2.74	2.58	

Table S7. The most possible dissociation channels and the corresponding dissociation energies (eV) of the  $\text{Al}_n\text{Sb}^q$  ( $q=0,-1$ ,  $n=1-16$ ) clusters.

clusters	DC	$E_D$	clusters	DC	$E_D$
$\text{AlSb}$	$\text{Al} + \text{Sb}$	1.58	$\text{AlSb}^-$	$\text{Al}^- + \text{Sb}$	3.07
$\text{Al}_2\text{Sb}$	$\text{Al} + \text{AlSb}$	2.49	$\text{Al}_2\text{Sb}^-$	$\text{Al} + \text{AlSb}^-$	2.80
$\text{Al}_3\text{Sb}$	$\text{Al} + \text{Al}_2\text{Sb}$	2.84	$\text{Al}_3\text{Sb}^-$	$\text{Al} + \text{Al}_2\text{Sb}^-$	2.53
$\text{Al}_4\text{Sb}$	$\text{Al} + \text{Al}_3\text{Sb}$	1.94	$\text{Al}_4\text{Sb}^-$	$\text{Al} + \text{Al}_3\text{Sb}^-$	2.11
$\text{Al}_5\text{Sb}$	$\text{Al} + \text{Al}_4\text{Sb}$	3.01	$\text{Al}_5\text{Sb}^-$	$\text{Al} + \text{Al}_4\text{Sb}^-$	3.17
$\text{Al}_6\text{Sb}$	$\text{Al} + \text{Al}_5\text{Sb}$	2.39	$\text{Al}_6\text{Sb}^-$	$\text{Al} + \text{Al}_5\text{Sb}^-$	2.34
$\text{Al}_7\text{Sb}$	$\text{Al} + \text{Al}_6\text{Sb}$	2.51	$\text{Al}_7\text{Sb}^-$	$\text{Al} + \text{Al}_6\text{Sb}^-$	2.77
$\text{Al}_8\text{Sb}$	$\text{Al} + \text{Al}_7\text{Sb}$	2.92	$\text{Al}_8\text{Sb}^-$	$\text{Al} + \text{Al}_7\text{Sb}^-$	2.87
$\text{Al}_9\text{Sb}$	$\text{Al} + \text{Al}_8\text{Sb}$	2.80	$\text{Al}_9\text{Sb}^-$	$\text{Al} + \text{Al}_8\text{Sb}^-$	2.48
$\text{Al}_{10}\text{Sb}$	$\text{Al} + \text{Al}_9\text{Sb}$	2.31	$\text{Al}_{10}\text{Sb}^-$	$\text{Al} + \text{Al}_9\text{Sb}^-$	2.81
$\text{Al}_{11}\text{Sb}$	$\text{Al} + \text{Al}_{10}\text{Sb}$	2.91	$\text{Al}_{11}\text{Sb}^-$	$\text{Al} + \text{Al}_{10}\text{Sb}^-$	3.34
$\text{Al}_{12}\text{Sb}$	$\text{Al} + \text{Al}_{11}\text{Sb}$	3.40	$\text{Al}_{12}\text{Sb}^-$	$\text{Al} + \text{Al}_{11}\text{Sb}^-$	2.75
$\text{Al}_{13}\text{Sb}$	$\text{Al} + \text{Al}_{12}\text{Sb}$	2.71	$\text{Al}_{13}\text{Sb}^-$	$\text{Al}_{13}^- + \text{Sb}$	2.26
$\text{Al}_{14}\text{Sb}$	$\text{Al} + \text{Al}_{13}\text{Sb}$	3.09	$\text{Al}_{14}\text{Sb}^-$	$\text{Al} + \text{Al}_{13}\text{Sb}^-$	3.23
$\text{Al}_{15}\text{Sb}$	$\text{Al} + \text{Al}_{14}\text{Sb}$	2.69	$\text{Al}_{15}\text{Sb}^-$	$\text{Al} + \text{Al}_{14}\text{Sb}^-$	2.16
$\text{Al}_{16}\text{Sb}$	$\text{Al} + \text{Al}_{15}\text{Sb}$	1.85	$\text{Al}_{16}\text{Sb}^-$	$\text{Al} + \text{Al}_{15}\text{Sb}^-$	2.20

Table S8. The most possible dissociation channels and the corresponding dissociation energies (eV) of  $\text{Al}_{n+1}^q$  ( $q=0,-1$ ,  $n=1-16$ ) clusters.

clusters	DC	$E_D$	clusters	DC	$E_D$
$\text{Al}_2$	$\text{Al} + \text{Al}$	1.45	$\text{Al}_2$	$\text{Al} + \text{Al}$	2.49
$\text{Al}_3$	$\text{Al} + \text{Al}_2$	2.15	$\text{Al}_3$	$\text{Al} + \text{Al}_2$	2.37
$\text{Al}_4$	$\text{Al} + \text{Al}_3$	1.79	$\text{Al}_4$	$\text{Al} + \text{Al}_3$	2.45
$\text{Al}_5$	$\text{Al} + \text{Al}_4$	2.74	$\text{Al}_5$	$\text{Al} + \text{Al}_4$	2.46
$\text{Al}_6$	$\text{Al} + \text{Al}_5$	2.73	$\text{Al}_6$	$\text{Al} + \text{Al}_5$	3.12
$\text{Al}_7$	$\text{Al} + \text{Al}_6$	3.38	$\text{Al}_7$	$\text{Al} + \text{Al}_6$	2.98
$\text{Al}_8$	$\text{Al} + \text{Al}_7$	2.20	$\text{Al}_8$	$\text{Al} + \text{Al}_7$	2.35
$\text{Al}_9$	$\text{Al} + \text{Al}_8$	2.58	$\text{Al}_9$	$\text{Al} + \text{Al}_8$	2.94
$\text{Al}_{10}$	$\text{Al} + \text{Al}_9$	2.63	$\text{Al}_{10}$	$\text{Al} + \text{Al}_9$	2.62
$\text{Al}_{11}$	$\text{Al} + \text{Al}_{10}$	2.76	$\text{Al}_{11}$	$\text{Al} + \text{Al}_{10}$	2.84
$\text{Al}_{12}$	$\text{Al} + \text{Al}_{11}$	2.98	$\text{Al}_{12}$	$\text{Al} + \text{Al}_{11}$	2.82
$\text{Al}_{13}$	$\text{Al} + \text{Al}_{12}$	3.41	$\text{Al}_{13}$	$\text{Al} + \text{Al}_{12}$	4.28
$\text{Al}_{14}$	$\text{Al} + \text{Al}_{13}$	2.82	$\text{Al}_{14}$	$\text{Al} + \text{Al}_{13}$	1.94
$\text{Al}_{15}$	$\text{Al} + \text{Al}_{14}$	2.45	$\text{Al}_{15}$	$\text{Al} + \text{Al}_{14}$	2.70
$\text{Al}_{16}$	$\text{Al} + \text{Al}_{15}$	2.83	$\text{Al}_{16}$	$\text{Al} + \text{Al}_{15}$	2.69
$\text{Al}_{17}$	$\text{Al} + \text{Al}_{16}$	2.69	$\text{Al}_{17}$	$\text{Al} + \text{Al}_{16}$	2.77

Table S9. The natural charge (NC) of Sb atom, the local magnetic moments of the 5s and 5p states for Sb atom, 3s and 3p states for Al atom in the most stable structures of  $\text{Al}_n\text{Sb}^q$  ( $q=0,-1$ ,  $n=1-16$ ) clusters, together with the total magnetic moments.

Size(n)	$\text{Al}_n\text{Sb}$						$\text{Al}_n\text{Sb}$					
	Sb	$\text{Sb}(M/\mu_B)$		$\text{Al}(M/\mu_B)$		Tot.	Sb	$\text{Sb}(M/\mu_B)$		$\text{Al}(M/\mu_B)$		Tot.
	NC(e)	5s	5p	3s	3p	( $\mu_B$ )	NC	5s	5p	3s	3p	( $\mu_B$ )
1	-0.34	0.00	1.46	0.15	0.38	2.01	-0.81	-0.01	0.48	0.14	0.45	1.08
2	-0.48	0.00	0.50	0.22	0.30	1.00	-1.13	0.00	0.00	0.00	0.00	0.00
3	-0.55	0.00	0.00	0.00	0.00	0.00	-0.58	0.01	0.09	0.05	0.85	1.02
4	-0.81	0.01	-0.02	0.06	0.92	0.93	-0.50	0.00	0.00	0.00	0.00	0.00
5	-0.27	0.00	0.00	0.00	0.00	0.00	-0.29	-0.01	0.22	0.16	0.66	1.03
6	-0.09	0.00	0.21	0.18	0.61	0.98	-0.29	0.00	0.00	0.00	0.00	0.00
7	-0.06	0.00	0.00	0.00	0.00	0.00	-0.33	-0.01	0.20	0.28	0.50	0.94
8	-0.13	0.01	-0.03	0.23	0.82	1.04	-0.28	0.00	0.00	0.00	0.00	0.00
9	-0.02	0.00	0.00	0.00	0.00	0.00	-0.21	0.00	0.03	0.19	0.76	0.98
10	-0.09	0.01	-0.02	0.23	0.76	0.95	-0.16	0.00	0.00	0.00	0.00	0.00
11	0.01	0.00	0.00	0.00	0.00	0.00	-0.13	0.01	-0.04	0.29	0.73	1.04
12	0.04	0.00	0.16	0.26	0.62	1.10	-0.11	0.00	0.00	0.00	0.00	0.00
13	0.04	0.00	0.00	0.00	0.00	0.00	-0.12	0.00	0.26	0.24	0.53	0.98
14	0.01	-0.01	0.20	0.33	0.40	0.96	-0.15	0.00	0.00	0.00	0.00	0.00
15	0.02	0.00	0.00	0.00	0.00	0.00	-0.12	0.00	0.00	0.24	0.70	0.94
16	-0.09	0.00	0.05	0.17	0.71	0.95	-0.22	0.00	0.00	0.00	0.00	0.00

## References:

- [1] J. J. Melko, P. A. Clayborne, C. E. Jones Jr., J. U. Reveles, U. Gupta, S. N. Khanna, and A. W. Castleman Jr., *J. Phys. Chem. A* **114**, 2045 (2010).
- [2] X. D. Xing, J. J. Wang, X. Y. Kuang, X. X. Xia, C. Lu, and G. Maroulis, *Phys. Chem. Chem. Phys.* **18**, 26177 (2016).
- [3] X. Li, H. B. Wu, X. B. Wang, L. S. Wang, *Phys. Rev. Lett.* **81**, 1909 (1998).
- [4] S. Paranthaman, K. Y. Hong, J. H. Kim, D. E. Kim, T. K. Kim, *J. Phys. Chem. A* **117**, 9293 (2013).