Supplementary Information

Quantum chemistry calculations of the growth patterns, simulated photoelectron spectra, and electronic properties of $LaASi_l$ (A = Sc, Y, La; $l \leqslant 10$) compounds and their anions

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Table S1. Bond Length and electronic state at the PBE method of dimers in comparison with the experimental value and other theoretical data.

	State	Bond Length		
		PBE	CASPT2/ANO-RCC[a]	Exp.[a]
La_2	$^1\Sigma_g$	2.605	2.692	2.8
Sc_2	$^5\Sigma_g$	2.599	2.745	
Y_2	$^5\Sigma_g$	2.943	3.011	

[a] Reference 56,57.

Table S2 AEAs and the relative energies(RE) (eV) of low-lying isomers of small

Clusters	AEAs		Isomers	RE	
	PBE	ROCCSD(T)		PBE	ROCCSD(T)
La_2Si	0.88	0.68	LES	0.00	0.00
La_2Si_2	1.10	0.97	LES	0.00	0.00
			2n1	0.06	0.16
$La_2Si_2^-$			LES	0.00	0.00
			2a1	0.36	0.65
La_2Si_3	0.81	0.77	LES	0.00	0.00
			3n1	1.18	0.99
$La_2Si_3^-$			LES	0.0	0.0
			4a1	0.53	0.51
LaYSi	0.88	0.67	LES	0.00	0.00
$LaYSi_2$	1.26	1.42	LES	0.0	0.0
			2n1	0.11	0.09
$LaYSi_2^-$			LES	0.00	0.00
			2a1	0.07	0.20
$LaYSi_3$	1.06	1.07	LES	0.0	0.0
			3n1	0.90	0.68
$LaYSi_3^-$			LES	0.00	0.00
			4a1	0.52	0.46
LaScSi	0.96	0.74	LES	0.0	0.0
$LaScSi_2$	1.27	1.45	LES	0.0	0.0
			2n1	0.09	0.06
$LaScSi_2^-$			LES	0.00	0.00
			2a1	0.06	0.15
$LaScSi_3$	1.04	1.02	LES	0.00	0.00
			3n1	0.90	0.72
			3n2	1.34	1.31
$LaScSi_3^-$			LES	0.00	0.00
			4a1	0.47	0.40
			4a2	0.86	0.92

$LaASi_l$((A = Sc, Y, and La; l$\leqslant$3) clusters.

Clusters	The position of electron binding energy						
	A	B	C	D	E	F	G
$LaScSi^-$	1.03	1.78	2.27	2.43			
$LaScSi_2^-$	1.57	1.37	2.16	2.48			
$LaScSi_3^-$	1.07	1.62	2.05	2.91			
$LaScSi_4^-$	2.06	2.3	2.87	3.09	3.5	3.88	4.11
$LaScSi_5^-$	1.82	2.51	2.87	3.19	3.68		
$LaScSi_6^-$	2.14	2.63	3.01	3.36	3.71		
$LaScSi_7^-$	2.53	2.98	3.5	3.98	4.26		
$LaScSi_8^-$	2.33	2.79	3.16	3.48	3.77	4.32	
$LaScSi_9^-$	2.82	3.4	3.78	4.14			
$LaScSi_{10}^-$	3.02	3.51	3.78	4.16			
$LaYSi^-$	0.97	1.75	2.27				
$LaYSi_2^-$	2.26	3	3.44	3.71			
$LaYSi_3^-$	1.09	1.58	2.02	2.85			
$LaYSi_4^-$	1.27	1.65	2.24	2.85	3.09	3.25	3.72
$LaYSi_5^-$	1.52	2.12	2.88	3.17	3.54	3.85	
$LaYSi_6^-$	1.84	2.32	3.17	3.49	4.15	4.34	
$LaYSi_7^-$	2.37	2.84	3.43	3.91			
$LaYSi_8^-$	2.08	2.53	2.98	3.41	4.04	4.34	
$LaYSi_9^-$	2.69	3.22	3.59	3.93	4.33		
$LaYSi_{10}^-$	2.25	2.92	3.91	4.36			
La_2Si^-	1.11	1.5	2.14	2.4			
$La_2Si_2^-$	1.28	2.19	2.45				
$La_2Si_3^-$	0.83	1.57	2.01	2.39	2.86		
$La_2Si_4^-$	2.53	2.91	3.06	3.66	3.82	4.28	

Table S3 The PES position of electron binding energy LES of anionic $LaASi_l$ ((A = Sc, Y, and La; $l \leq 10$) clusters.

$La_2Si_5^-$	2.28	2.88	3.35	3.6			
$La_2Si_6^-$	1.77	2.24	3.09	3.29	4.08	4.24	
$La_2Si_7^-$	2.32	2.78	3.37	3.82			
$La_2Si_8^-$	2.19	2.6	3.09	3.5	3.84	4.34	
$La_2Si_9^-$	2.21	2.68	3.05	3.64	4.15	4.32	
$La_2Si_{10}^-$	2.19	2.77	3.12	3.46	3.79	4.33	

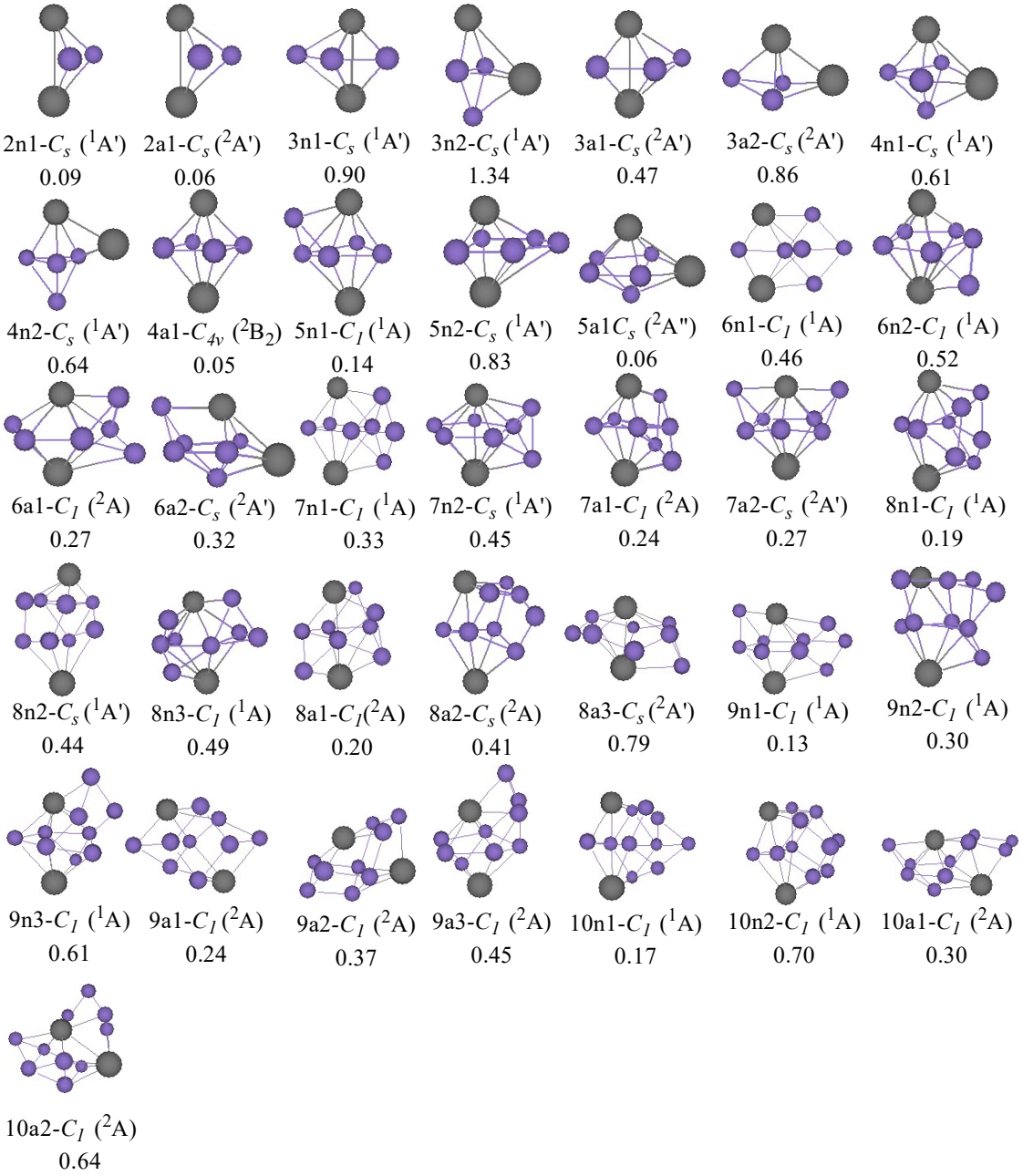

Figure S1 Part of isomers of $LaScSi_l$ clusters. The first value stands for l, n and a stand for neutral and anion. The upper gray balls are scandium, purple ball are silicon atoms, and the gray on the bottom is lanthanum. The symmetry, electronic state (in parentheses) and relative energy are given below the structure for each size.

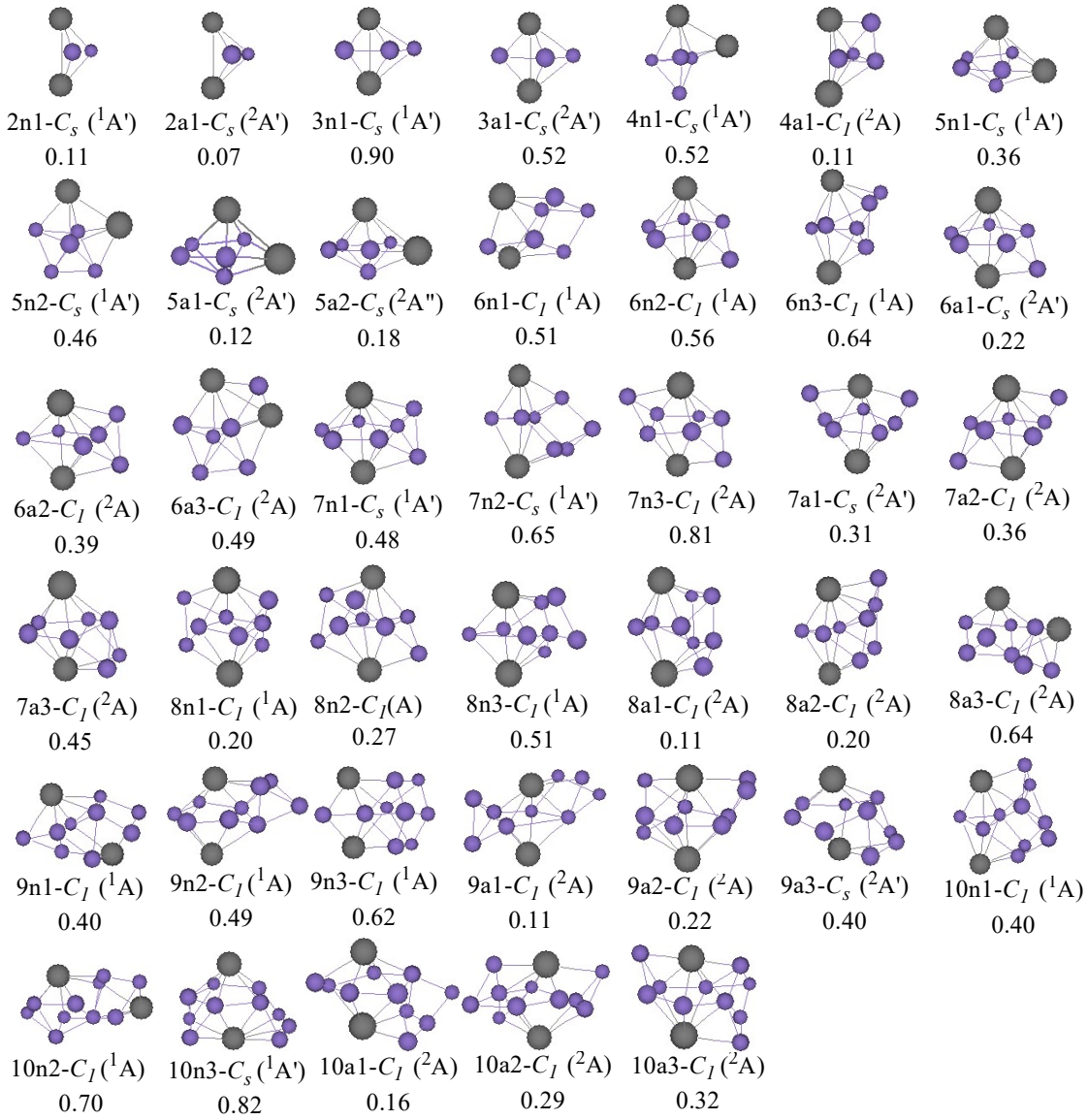

Figure S2 Part of isomers of $LaYSi_l$ clusters. The first value stands for l, n and a stand for neutral and anion. The upper gray balls are yttrium; purple ball are silicon atoms, and the gray on the bottom is lanthanum. The symmetry and electronic state (in parentheses) are given below the structure for each size. The symmetry, electronic state (in parentheses) and relative energy are given below the structure for each size.

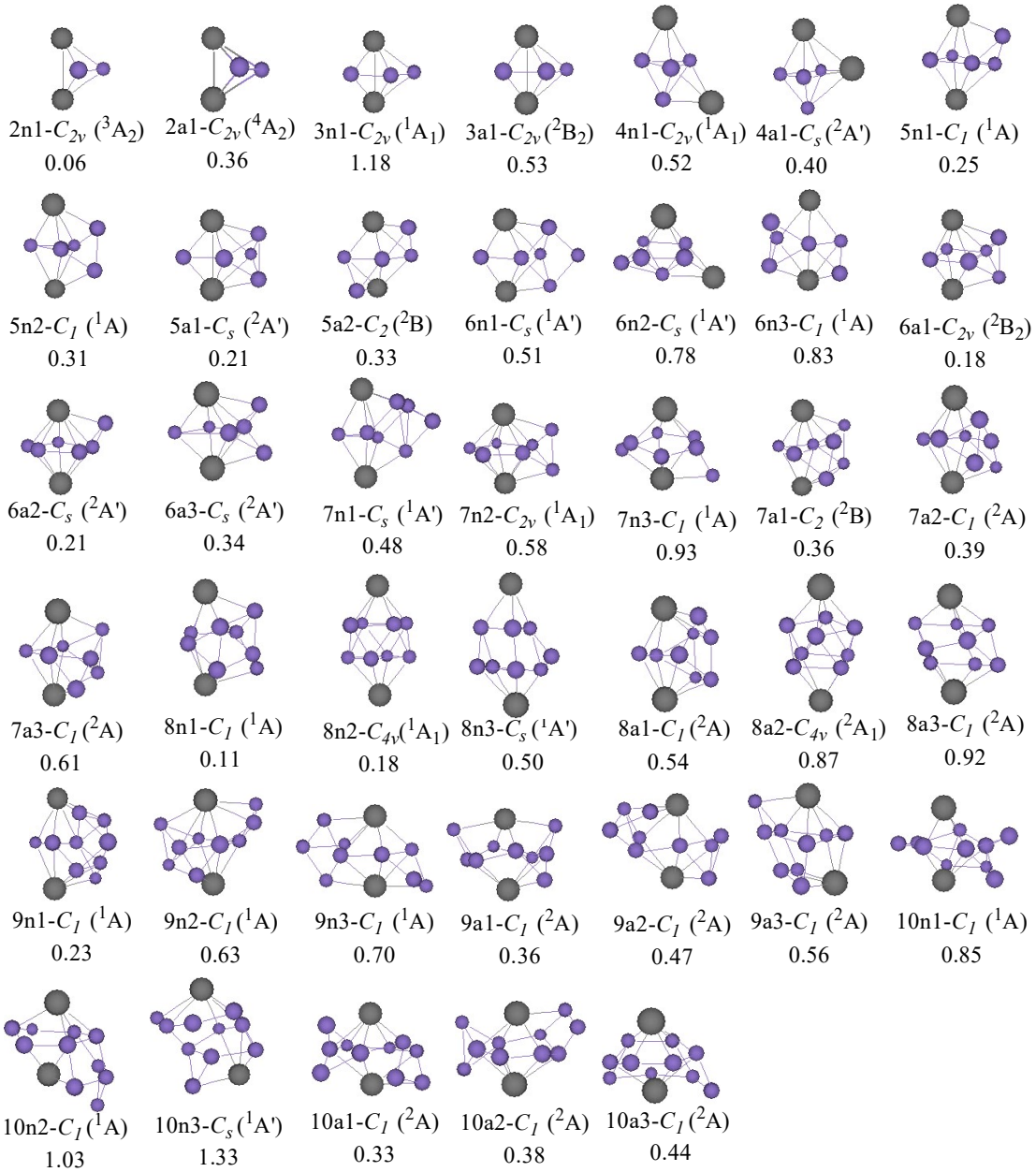

Figure S3 Part of isomers of La_2Si_l clusters. The first value stands for l, n and a stand for neutral and anion. The gray on the bottom is lanthanum and purple ball are silicon atoms. The symmetry, electronic state (in parentheses) and relative energy are given below the structure for each size.