

## Supplementary Information

### Relatively stable, square bipyramidal structure of $Ti_2Si_4$ : structural probe and electronic properties of neutral and anionic $TiASi_l$ ( $A = Sc, Ti; l \leq 12$ )

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Table S1 The PES position of electron binding energy GMS of anionic  $\text{TiASi}_i$  ( $A = \text{Sc and Ti}; i \leq 12$ ) clusters.

Clusters	The position of electron binding energy							
	A	B	C	D	E	F	G	H
$\text{TiScSi}^-$	1.48	2.03	2.62					
$\text{TiScSi}_2^-$	1.51	1.78	2.7	3.02				
$\text{TiScSi}_3^-$	1.93	2.15	2.54	3.15	3.43	3.7		
$\text{TiScSi}_4^-$	2.17	2.51	3.15	3.34	3.61	3.91		
$\text{TiScSi}_5^-$	2.06	2.23	2.51	2.99	3.17	3.61	4.09	4.32
$\text{TiScSi}_6^-$	2.45	2.71	2.99	3.49	3.9			
$\text{TiScSi}_7^-$	2.84	3.46	3.76	4.09				
$\text{TiScSi}_8^-$	2.7	3.24	3.67	4.14	4.43			
$\text{TiScSi}_9^-$	3.39	3.6	4.25					
$\text{TiScSi}_{10}^-$	3.31	3.87	4.06					
$\text{TiScSi}_{11}^-$	2.86	3.08	3.39	3.79	4.11	4.44		
$\text{TiScSi}_{12}^-$	3.00	3.73	4.14					
$\text{Ti}_2\text{Si}^-$	1.52	1.92	2.16	2.63				
$\text{Ti}_2\text{Si}_2^-$	1.48	1.85	2.25	3.06				
$\text{Ti}_2\text{Si}_3^-$	2.58	2.79	3.32	3.83	4.08	4.45		
$\text{Ti}_2\text{Si}_4^-$	2.02	2.43	2.9	3.45	3.81	4.14		
$\text{Ti}_2\text{Si}_5^-$	2.8	3.11	3.76	4.07	4.39			
$\text{Ti}_2\text{Si}_6^-$	2.31	2.68	3.08	3.45	4			
$\text{Ti}_2\text{Si}_7^-$	2.74	3.11	3.31	4.36				
$\text{Ti}_2\text{Si}_8^-$	3.2	3.81	4.19	4.36				
$\text{Ti}_2\text{Si}_9^-$	3.36	3.89	4.35					
$\text{Ti}_2\text{Si}_{10}^-$	3.31	3.7	4.19	4.44				
$\text{Ti}_2\text{Si}_{11}^-$	3.5	3.84	4.27					
$\text{Ti}_2\text{Si}_{12}^-$	3.62	4.12	4.37					

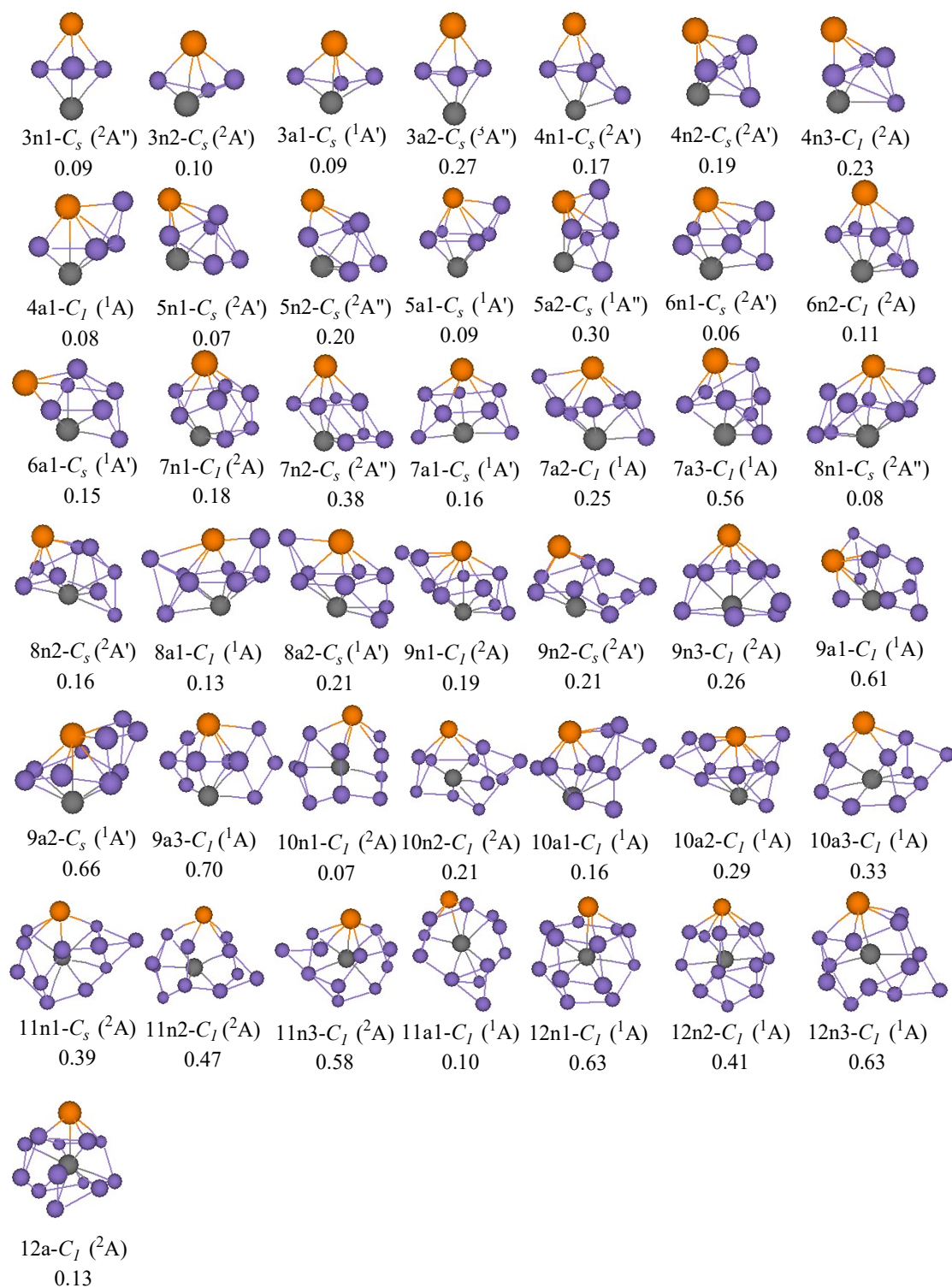


Figure S1 Part of isomers of TiScSi<sub>l</sub> clusters. The first value stands for l, n and a stand for neutral and anion. The orange balls are scandium, purple ball are silicon atoms, and the gray balls on the bottom are titanium atoms. The symmetry, electronic state (in parentheses) and relative energy are given below the structure for each size.

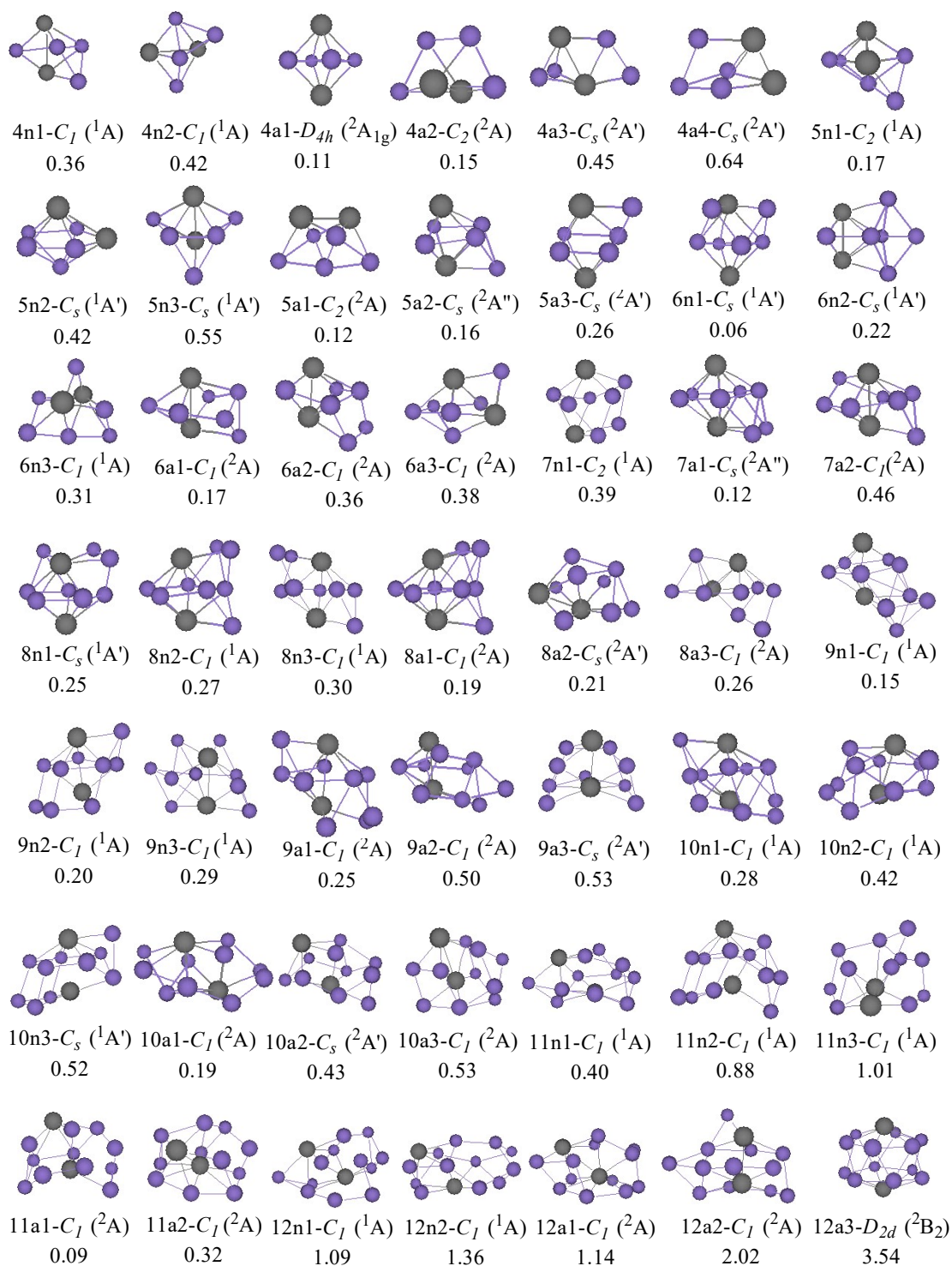


Figure S2 Part of isomers of  $Ti_2Si_l$  clusters. The first value stands for  $l$ ,  $n$  and a stand for neutral and anion. The upper gray balls are titanium atoms, purple ball are silicon atoms. The symmetry, electronic state (in parentheses) and relative energy are given below the structure for each size.