

Supporting Information

Structural and Bonding Properties of Small TiGe_n^- ($n = 2-6$) Clusters: Photoelectron Spectroscopy and Density Functional Calculations

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Table S1. Cartesian coordinates for stable isomers of TiGe_n^- ($n = 2-6$) clusters.

TiGe₂⁻						
2A				2B		
	X	Y	Z	X	Y	Z
Ge	0.00000000	1.26444200	-0.53794500	Ge	0.00000000	2.04992200
Ge	0.00000000	-1.26444200	-0.53794500	Ge	0.00000000	-0.20114900
Ti	0.00000000	0.00000000	1.56493100	Ti	0.00000000	-2.68912500

TiGe₃⁻						
	3A				3B	
	X	Y	Z	X	Y	Z
Ge	0.89107200	-1.26215200	-0.27798300	Ge	0.00000000	1.35608700
Ge	-1.58548400	-0.00099000	-0.49836000	Ge	0.00000000	-0.11145500
Ge	0.88815200	1.26419800	-0.27664500	Ge	0.00000000	-0.11145500
Ti	-0.28180400	-0.00153500	1.53162000	Ti	0.00000000	-1.64825600

TiGe₄⁻						
	4A				4B	
	X	Y	Z	X	Y	Z
Ge	0.00040000	-1.46065000	-0.61453400	Ge	-1.78476600	-0.24238100
Ge	0.00055700	1.46113600	-0.61398400	Ge	0.13110300	1.57018200
Ge	-1.99947800	-0.00003400	0.05464700	Ge	0.13110300	-1.57018200
Ge	1.99907700	-0.00014800	0.05540400	Ge	0.13110300	0.00000000
Ti	-0.00080900	-0.00044200	1.62686100	Ti	2.02393900	-0.02384100

4C		
Ge	-1.30496200	1.22000000
Ge	1.30501800	1.22000600
Ge	-2.52373700	-0.83231900
Ge	2.52368700	-0.83236800
Ti	-0.00000700	-1.12773500

TiGe₅⁻						
	5A				5B	
	X	Y	Z	X	Y	Z
Ge	0.00000000	0.00000000	1.68703300	Ge	-0.01269500	-1.37160300
Ge	0.00000000	1.93005400	-0.11202800	Ge	2.02060800	-0.00000300
Ge	0.00000000	-1.93005400	-0.11202800	Ge	-0.01269500	1.37161900
Ge	-1.93005400	0.00000000	-0.11202800	Ge	-2.17005900	-0.00000200
Ge	1.93005400	0.00000000	-0.11202800	Ge	1.11709600	-0.00000600
Ti	0.00000000	0.00000000	-1.80206900	Ti	-1.37055200	-0.00000800

5C		
Ge	1.06587000	-1.76458500
Ge	-0.27139000	-0.14153600

Ge	1.74218400	0.80002400	-0.00013000
Ge	-0.27147600	-0.14160700	-1.44828200
Ge	-0.63491800	1.94015400	-0.00002100
Ti	-2.37130200	-1.00720200	-0.00009300

TiGe₆

6A			6B				
X	Y	Z	X	Y	Z		
Ge	1.55728300	1.53350700	-0.13366300	Ge	-0.29888083	-1.18415764	2.15980078
Ge	-0.97831000	1.97380400	-0.06529200	Ge	-0.29888083	-1.18415764	-2.15980078
Ge	1.97281400	-0.94962900	-0.11911300	Ge	0.52575511	-2.21406793	0.00000000
Ge	-0.24402300	-2.17425000	-0.12352100	Ge	0.60700105	1.09004079	1.85074254
Ge	-2.17415400	-0.41077500	-0.02679400	Ge	0.60700105	1.09004079	-1.85074254
Ge	0.02270000	-0.00443200	1.58904700	Ge	-0.36945510	2.42559103	0.00000000
Ti	-0.22736000	0.04621900	-1.63005700	Ti	-1.12369899	-0.03718300	0.00000000

6C

Ge	2.61170500	-0.00042500	-0.47328700
Ge	-0.80521000	1.46218500	0.74986300
Ge	-0.80379500	-1.46357300	0.74856300
Ge	1.58036900	1.41537100	-0.72135000
Ge	1.28998100	0.00039200	1.46873800
Ge	1.58278400	-1.41368600	-0.72076500
Ti	-0.33807300	-0.00038300	-1.52983500