Supporting Information

Unusual Electronic and Bonding Properties of the Zintl Phase Ca_5Ge_3 and Related Compounds. A Theoretical Analysis

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Parameters used for the Hückel calculation

atom	orbital	H_{ii} (eV)	α_{ii}	c_1	α_{i2}	c_2
Ca [1]	4s	-6.111	1.2			
	4p	-4.219	1.2			
	3d	-5.0	4.0	0.4000	1.3	0.7000
Ge [2]	4s	-16.000	2.16	1.0000		
	4p	-9.0000	1.85	1.0000		

[1] T. D. Brennan, J. K. Burdet, Inorg. Chem. 32, 746 (1993)

[2] Ren, J.; Liang, W.; Whangbo, M.-H., CAESAR, PrimeColor Software Inc., Raleigh, NC, USA, 1998.

Crystallographic data for Ca_5Ge_3 [3]

	tetragonal
Crystal system	
Space group	$I4/mcm$ (no. 140)
Unit cell dimensions	$a = 7.7156(5) \text{ \AA}$
	$c = 14.885(2) \text{ \AA}$
Z	4
Pearson code	tI32
Wyckoff sequence	lhca

Atomic positions in Ca_5Ge_3

Atom	Wyck.	x	y	z
Ca 1	4c	0	0	0
Ca 2	16l	0.17807(8)	$x + 1/2$	0.13998(6)
Ge 1	4a	0	0	1/4
Ge 2	8h	0.38200(6)	$x + 1/2$	0

[3] E. A. Leon-Escamilla, J. D. Corbett, J. Solid State Chem. 2001, 159, 149.

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Figure S1. Band structure (left) and density of states (right) for Ca_6Ge_3 obtained from LMTO-ASA calculations. Dashed line signifies the Fermi level.

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Figure S2. Band structure for Ca_5Ge_3 obtained from FP-APW calculations in the fatband representation for Ge1 p_x (left) and Ge1 p_y (right).