Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

High electron affinity triggered by lithium coordination: quasi-chalcogen properties of Li_2Sn_8Be

Duomei Xue,[a] Zeren Chen,[b] Jingyao Liu,[a] Di Wu,[a] Zhiru Li[a], Ying Li*[a]

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* Corresponding author.
E-mail address: liyingedu@ jlu.edu.cn (Y. Li).
[a]Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, College of Chemistry, Jilin University, Changchun 130023, PR China
[b]School of Mechanical and Aerospace Engineering, Jilin University, Changchun 130025, PR China

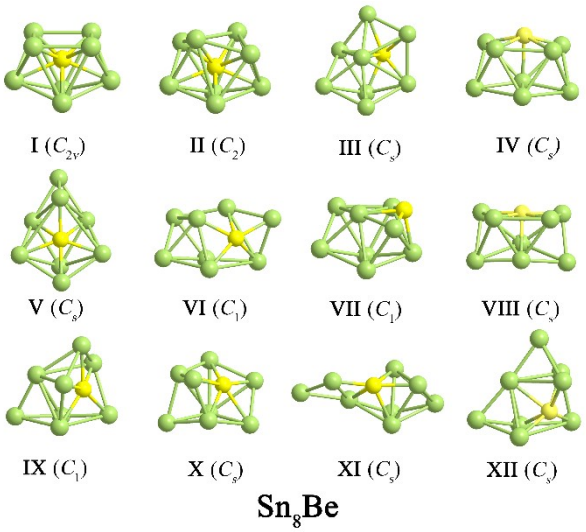

Figure S1. Optimized geometries of Sn_8Be. Symmetry point groups are given in the parentheses.

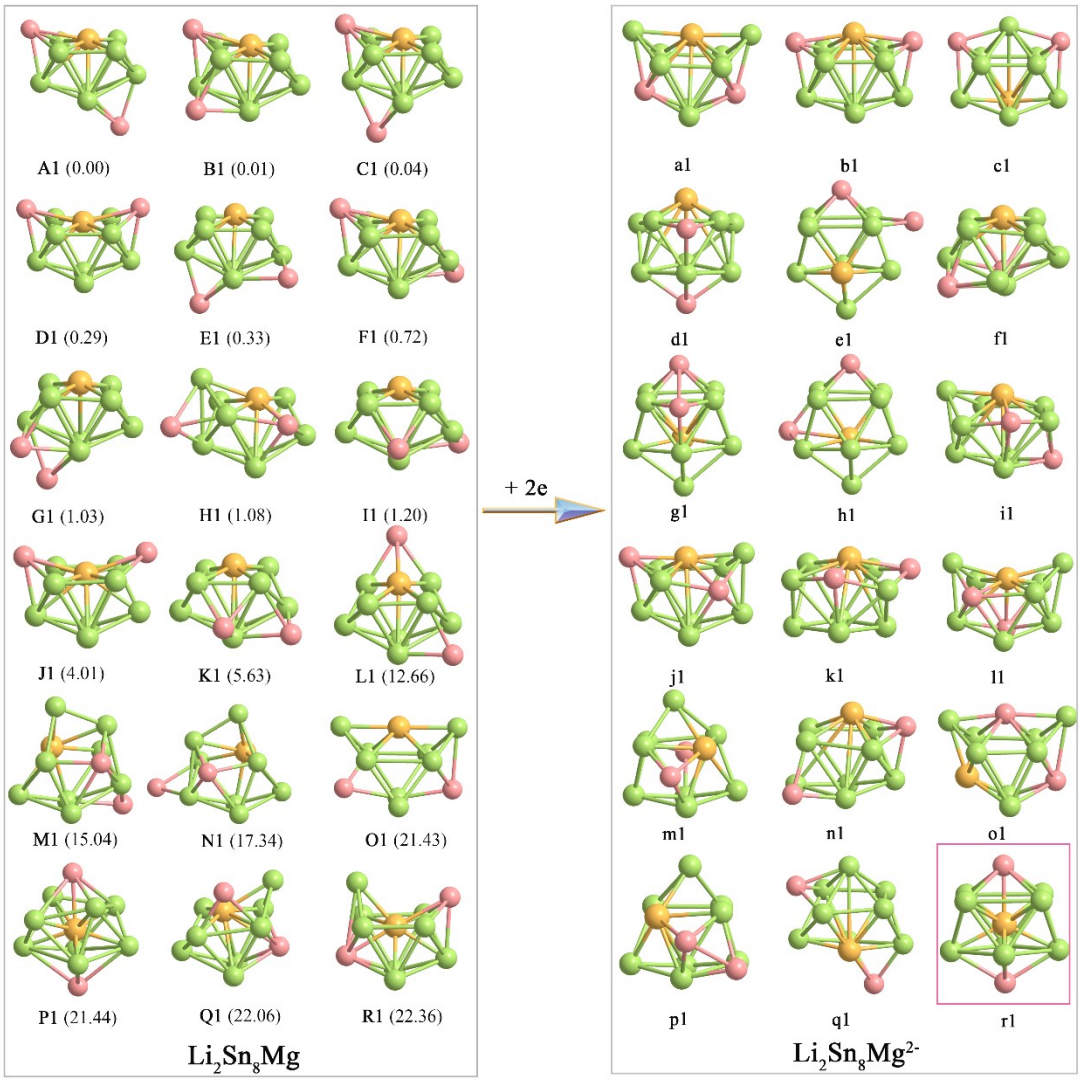

Figure S2. Low-lying isomers of Li_2Sn_8Mg and their corresponding $Li_2Sn_8Mg^{2-}$ clusters. Relative energies (in kcal mol^{-1}) are given in parentheses.

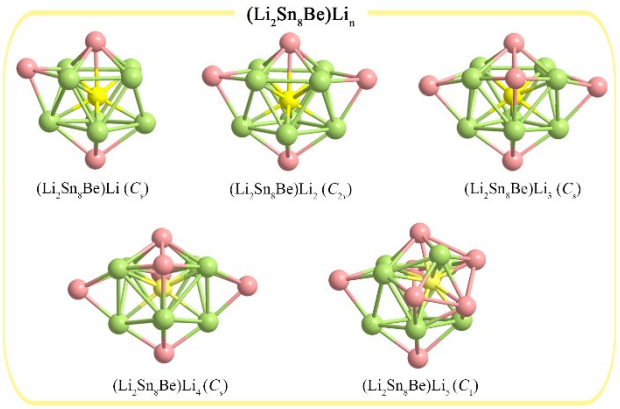

Figure S3. Optimized structures of $(Li_2Sn_8Be)Li_n$ (n = 1-5) with point group symmetry in parentheses.

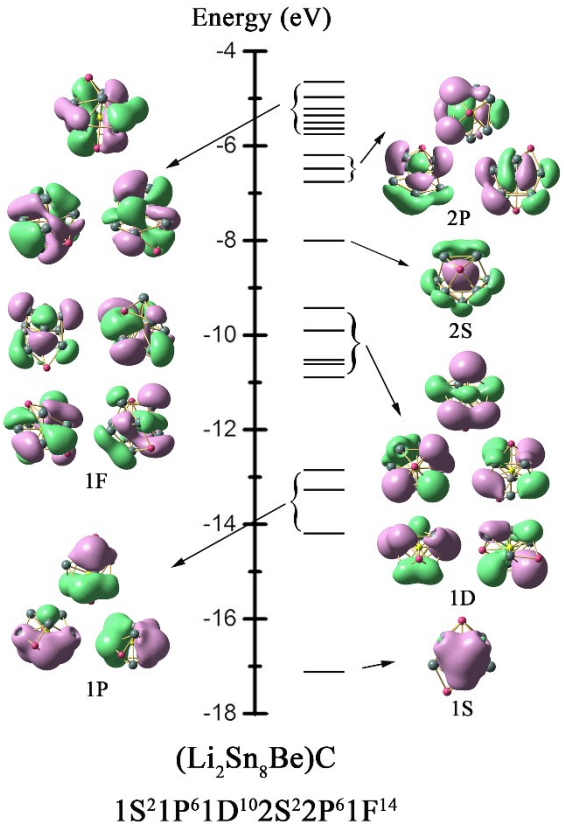

Figure S4. Electron-shell structure of the $(Li_2Sn_8Be)C$ cluster.

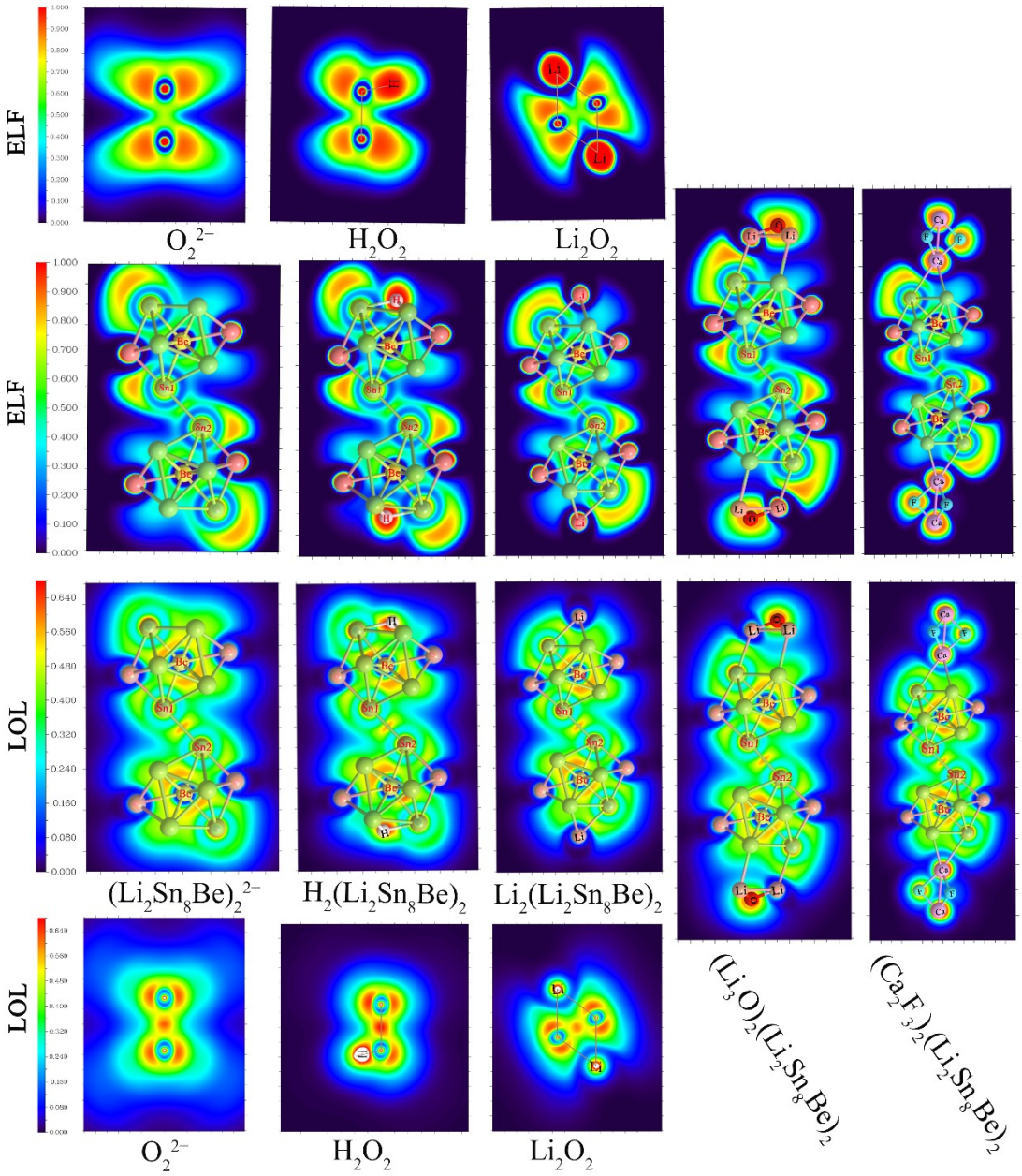

Figure S5. Cut-plane ELF and LOL maps of the $(Li_2Sn_8Be)_2^{2-}$, $H_2(Li_2Sn_8Be)_2$, $Li_2(Li_2Sn_8Be)_2$, $(Li_3O)_2(Li_2Sn_8Be)_2$, and $(Ca_2F_3)_2(Li_2Sn_8Be)_2$ compounds.

Table S1. Relative Energies (E_{rel}, in kcal mol^{-1}), Symmetry Point Groups, Average Binding Energies (E_a, in eV), Number of Be-Sn Bonds (N), Average Be-Sn Bond Lengths (R_0, in Å), and HOMO − LUMO Gaps (in eV) of the Sn_8Be isomers.

Isomer	E_{rel}	symmetry	E_a	gap	N	R_0
I	0.00	C_{2v}	4.07	2.45	8	2.615
II	0.95	C_2	4.06	2.23	8	2.593
III	22.22	C_s	3.97	1.76	6	2.641
IV	22.98	C_s	3.96	1.98	5	2.604
V	24.28	C_s	3.95	1.69	7	2.641
VI	29.57	C_1	3.92	1.80	6	2.642
VII	30.36	C_1	3.92	1. 87	4	2.510
VIII	30.81	C_s	3.92	2.11	6	2.637
IX	34.41	C_1	3.90	1.98	6	2.617
X	43.71	C_s	3.86	1.74	6	2.687
XI	44.49	C_s	3.85	1.76	5	2.606
XII	47.41	C_s	3.84	1.76	6	2.623

Table S2. Symmetry Point Groups, and Important Geometrical Parameters (in Å), and Average Binding Energies (in eV) of the concerned $[Li_2Sn_8]^{4-}$, Li_2Sn_8Be, $Li_2Sn_8Be^{2-}$, Li_2Sn_8Mg, and $Li_2Sn_8Mg^{2-}$ Clusters.

	symmetry	R_0	w	h	E_a
$[Li_2Sn_8]^{4-}$	D_{4d}	2.653	4.703	2.455	
Li_2Sn_8Be	D_{4d}	2.652	4.716	2.430	3.68
$Li_2Sn_8Be^{2-}$	D_{4d}	2.651	4.700	2.456	
Li_2Sn_8Mg	D_{4d}	2.821	5.088	2.438	3.34
$Li_2Sn_8Mg^{2-}$	D_{4d}	2.813	5.049	2.482	

Table S3. Average Binding Energies of Li atom (E_b, in eV), the Second Difference in Energy (Δ^2E, in eV), Dissociation Energies (ΔE, in eV), and HOMO–LUMO Gaps of the $(Li_2Sn_8Be)Li_n$ (n = 1-5) Compounds.

Isomers	E_b	ΔE	Δ^2E	Gap/eV
$(Li_2Sn_8Be)Li$	2.328	2.328	−0.937	1.40
$(Li_2Sn_8Be)Li_2$	2.527	2.726	2.014	2.53
$(Li_2Sn_8Be)Li_3$	1.922	0.713	−0.585	1.54
$(Li_2Sn_8Be)Li_4$	1.766	1.297	0.167	1.53
$(Li_2Sn_8Be)Li_5$	1.639	1.130		1.47

Table S4. The binding energies (E_b^M) and HOMO–LUMO gaps of the $(Li_2Sn_8Be)M$ (M = Li, Be, B, C, N, O, and F) compounds.

Species	E_b^M /kcal mol^{-1}	Gap/ eV
$(Li_2Sn_8Be)Li$	53.7	1.40
$(Li_2Sn_8Be)Be$	80.5	2.10
$(Li_2Sn_8Be)B$	114.3	1.87
$(Li_2Sn_8Be)C$	199.4	2.21
$(Li_2Sn_8Be)N$	171.3	1.52
$(Li_2Sn_8Be)O$	163.9	1.91
$(Li_2Sn_8Be)F$	67.8	1.60