Electronic supporting information for:

Insight into $Y@X_2B_8$ (Y= Li, CO_2 and Li-CO_2, X = Be, B and C) nanostructures: A computational study

Table S1 The interatomic distance (Å) and the values of the electron density ($\rho(r)$) and $\nabla^2\rho$(r) (in a.u.) in the interaction between the Li atom and other atoms

Species	quantity	Interaction	Interatomic distance (Å)	$\rho(r)$	$\nabla^2\rho(r)$
Be_2B_8-Li-α	1	Li-B	2.07	0.0270	0.1419
Be_2B_8-Li-β	2	Li-B	2.39	0.0179	0.0861
	1	Li-Be	2.45	0.0141	0.0406
B_2B_8-Li-α	2	Li-B	2.39	0.0151	0.0926
B_2B_8-Li-β	1	Li-B	2.21	0.0255	0.1208
Be_2B_8-Li-γ	1	Li-B	2.13	0.0235	0.1258
C_2B_8-Li	2	Li-C	2.23	0.0183	0.1310

Table S2 The energies of E_1 and E_2 (in Hartree), the adsorption and the vertical ionization (VI) energies (in eV) at the (P)MP2/aug-cc-pVDZ//UMP2/6-311+G(d) level

Species	E_1	E_2	Adsorption energy	VI
Be_2B_8-Li-α	-234.76841	-234.51210	-1.52	6.97
Be_2B_8-Li-β	-234.77706	-234.51948	-1.76	7.01
B_2B_8-Li-α	-254.90112	-254.63690	-3.05	7.19
B_2B_8-Li-β	-254.87324	-254.61166	-2.29	7.12
B_2B_8-Li-γ	-254.88695	-254.62901	-2.66	7.02
C_2B_8-Li	-281.24473	-280.99138	-1.61	6.89

The E_1 stands for the energy of the Li@X_2B_8 (X=Be, B and C) species through optimization process.

The E_2 stands for the energy of the $[Li@X_2B_8\ (X = Be, B \text{ and } C)]^+$ species through the calculation of single-point energy.

The adsorption and the vertical ionization (VI) energies have been calculated by $E_1 – E(Li) – E$ (Be_2B_8 or B_2B_8 or C_2B_8) and E_2-E_1, respectively

Table S3 The HOMO and the LUMO energies and the HOMO-LUMO energy gaps for all reported molecules

Species	Set α		Set β		HOMO-LUMO energy gap
	HOMO orbital energy	LUMO orbital energy	HOMO orbital energy	LUMO orbital energy	
Be_2B_8	*-8.53*	*-0.04*			8.49
Be_2B_8-Li-α	-7.31	-0.38	*-7.25*	*-0.41*	6.84
Be_2B_8-Li-β	*-7.16*	-0.07	-8.00	*-0.12*	7.04
B_2B_8	*-8.72*	*-0.82*			7.90
B_2B_8-Li-α	-7.68	-0.09	*-7.65*	*-0.16*	7.49
B_2B_8-Li-β	*-6.78*	-0.69	-6.78	*-0.70*	6.08
Be_2B_8-Li-γ	*-7.04*	*-0.47*	-7.05	-0.47	6.57
C_2B_8	*-7.50*	*0.21*			7.71
C_2B_8-Li	*-6.92*	0.14	-7.31	*-0.33*	6.59

All energies are in eV

Italic values have been used in the calculation of the HOMO-LUMO energy gap

Table S4 NBO charges of all the atoms in the Li@X_2B_8 (X = Be, B and C) molecules

Atoms	Species					
	Be_2B_8-Li-α	Be_2B_8-Li-β	B_2B_8-Li-α	B_2B_8-Li-β	Be_2B_8-Li-γ	C_2B_8-Li
B1	0.08	-0.19	-0.04	0.13	-0.19	0.04
B2	-0.35	-0.24	-0.16	-0.13	-0.35	0.04
B3	-0.31	-0.26	-0.04	0.06	-0.19	0.09
B4	-0.33	-0.28	-0.04	0.01	0.04	0.09
B5	-0.24	-0.20	-0.04	0.09	0.07	0.04
B6	-0.28	-0.22	-0.16	-0.12	-0.16	0.05
B7	-0.49	-0.36	-0.04	-0.28	0.07	0.09
B8	-0.94	-0.36	-0.04	-0.26	0.04	0.09
B9	----	----	-0.13	-0.14	-0.12	----
B10	----	----	-0.13	-0.27	-0.12	----
Be1	0.97	0.43	----	----	----	----
Be2	0.99	0.87	----	----	----	----
C1	----	----	----	----	----	-0.66
C2	----	----	----	----	----	-0.65
Li	0.90	0.81	0.80	0.91	0.90	0.76

Table S5 The first hyperpolarizability (β_{total}) and its components for all the $Li@X_2B_8$ (X = Be, B and C) molecules (a.u)

Components	Species					
	Be_2B_8-Li-α	Be_2B_8-Li-β	B_2B_8-Li-α	B_2B_8-Li-β	Be_2B_8-Li-γ	C_2B_8-Li
β_{total}	1085	1257	50	2200	457	1079
β_{xxx}	1168	407	0	2677	26	0
β_{xxy}	-131	0	0	866	-236	0
β_{xyy}	289	131	0	591	-13	0
β_{yyy}	-722	0	13	171	-315	0
β_{xxz}	210	-236	-39	-144	-131	79
β_{yyz}	13	-26	131	53	79	-236
β_{xzz}	66	696	-13	197	-13	0
β_{yzz}	-92	0	13	157	-210	0
β_{zzz}	26	-1430	-13	-26	92	-1640
β_x	913	740	-8	2079	0	0
β_y	-567	0	16	716	-457	0
β_z	150	-1016	47	-71	24	-1079