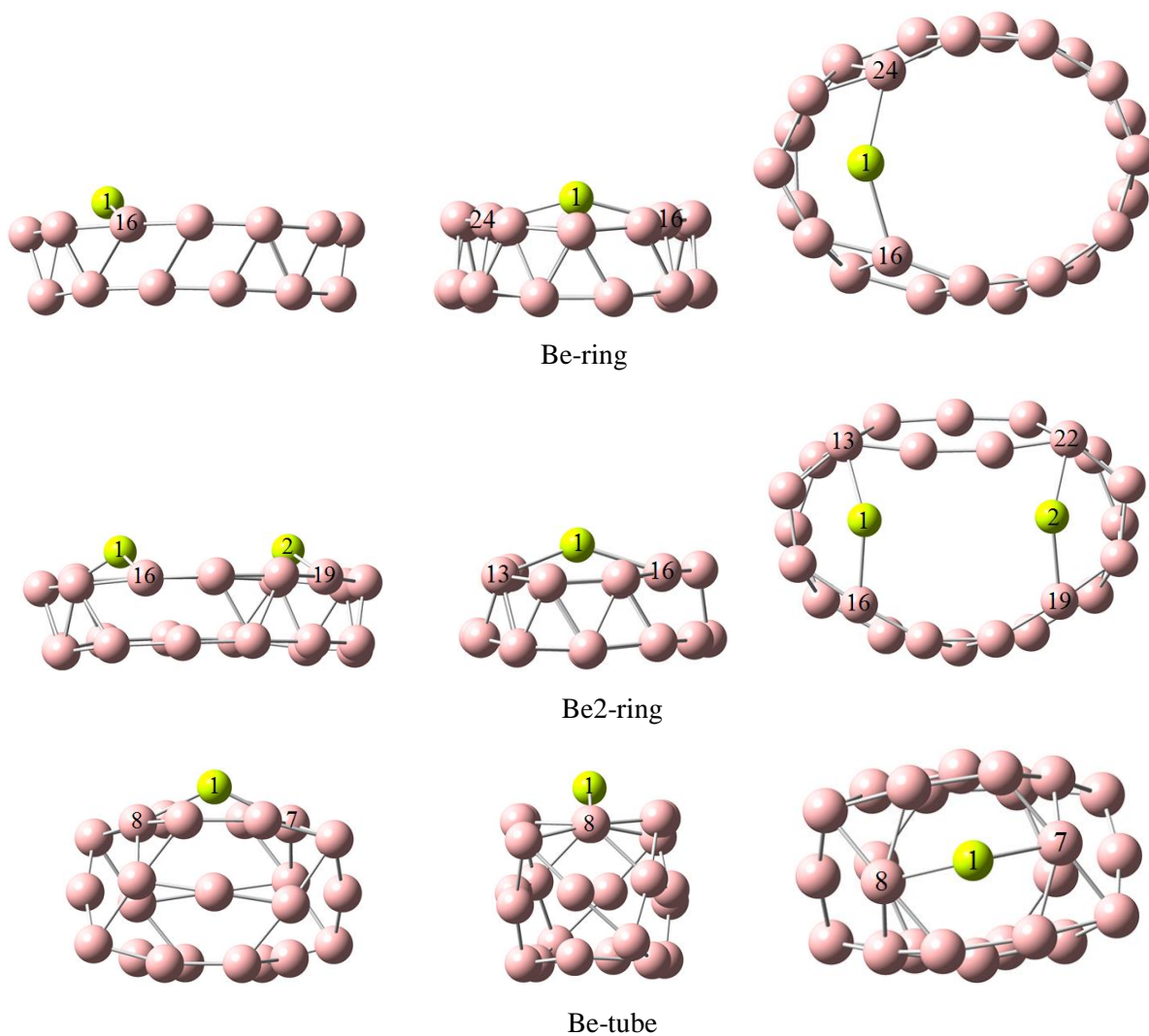
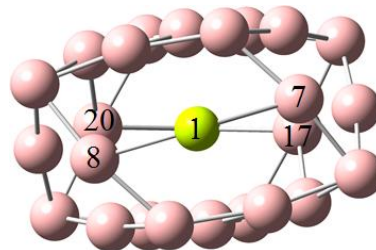
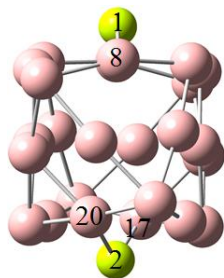
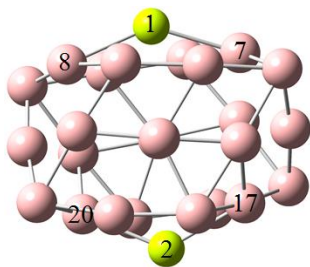
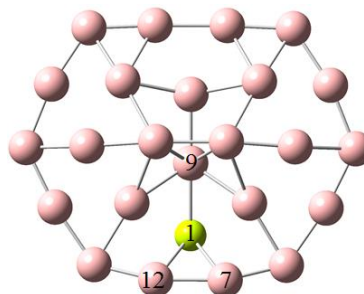
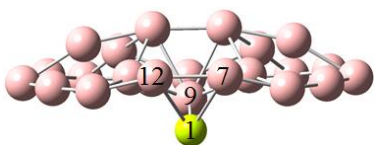


Be doping: An effective way to improve the Li-atom adsorption
in boron rich nanoflake of B₂₄

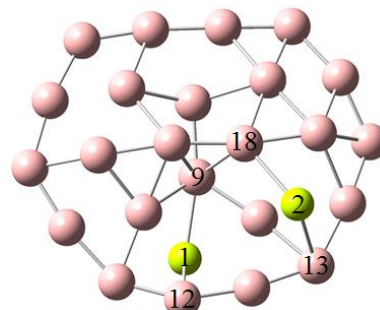
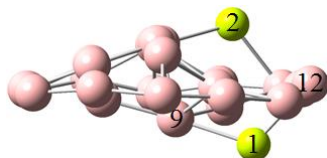
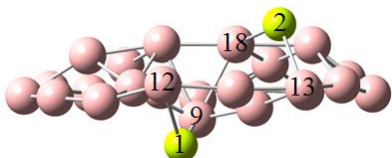




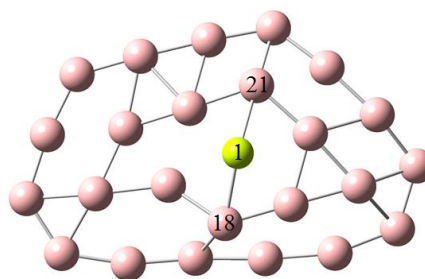
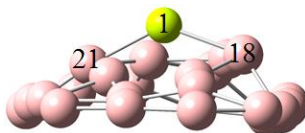
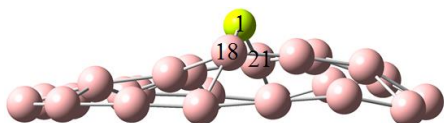
Be2-tube



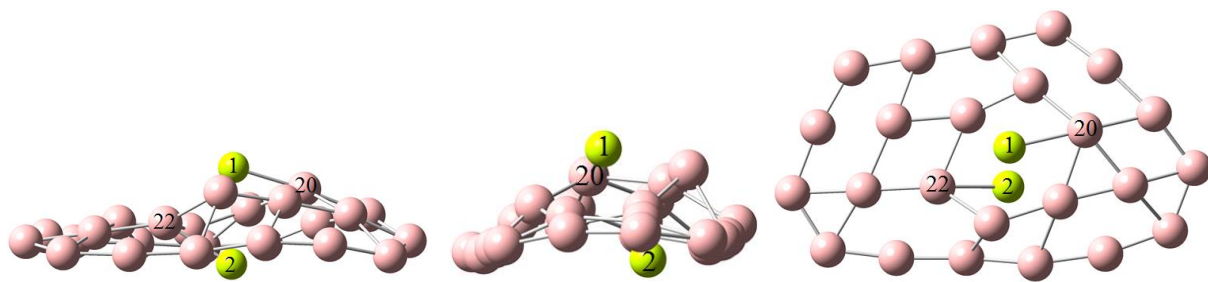
Be-convex



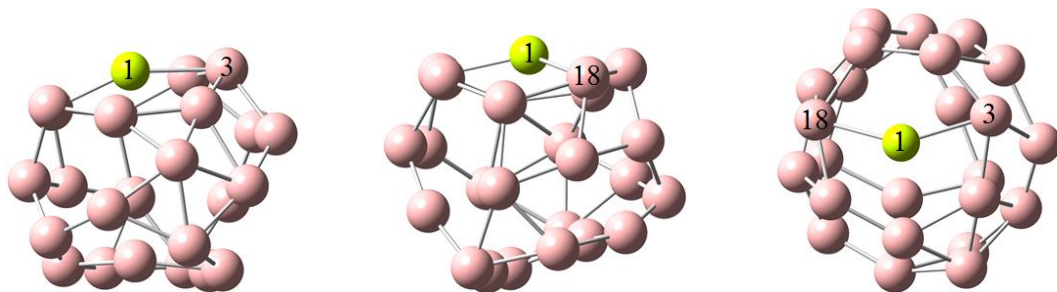
Be2-convex



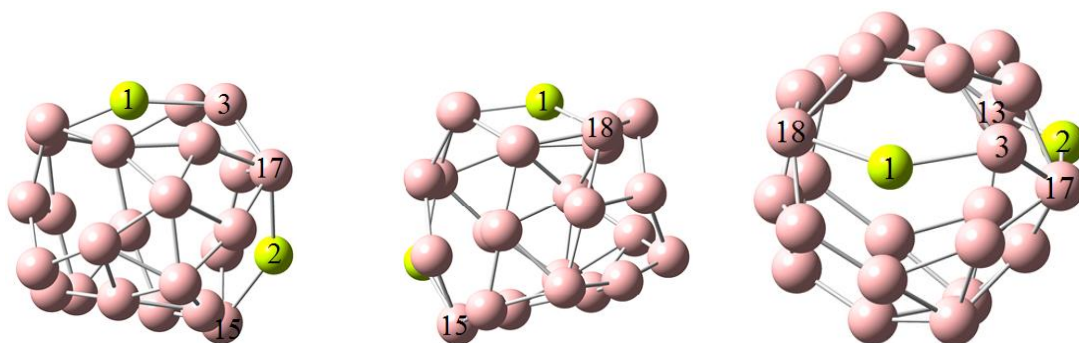
Be-quasiplanar



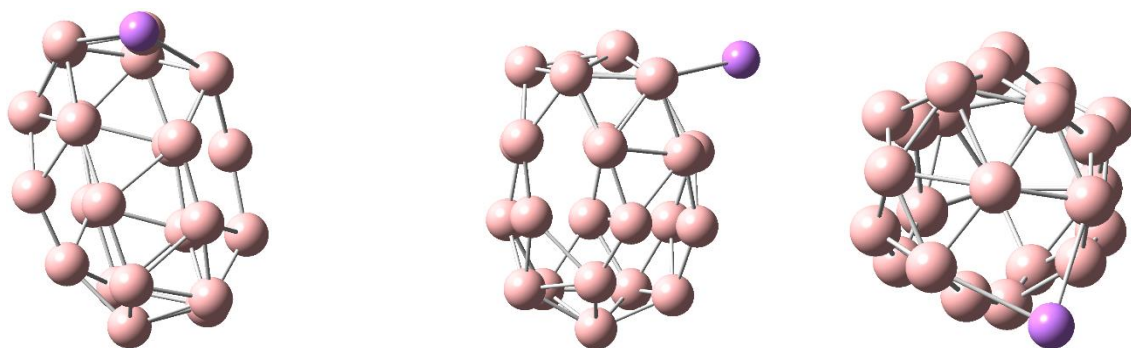
Be2-quasiplanar



Be-cage



Be2-cage



Cage-Li

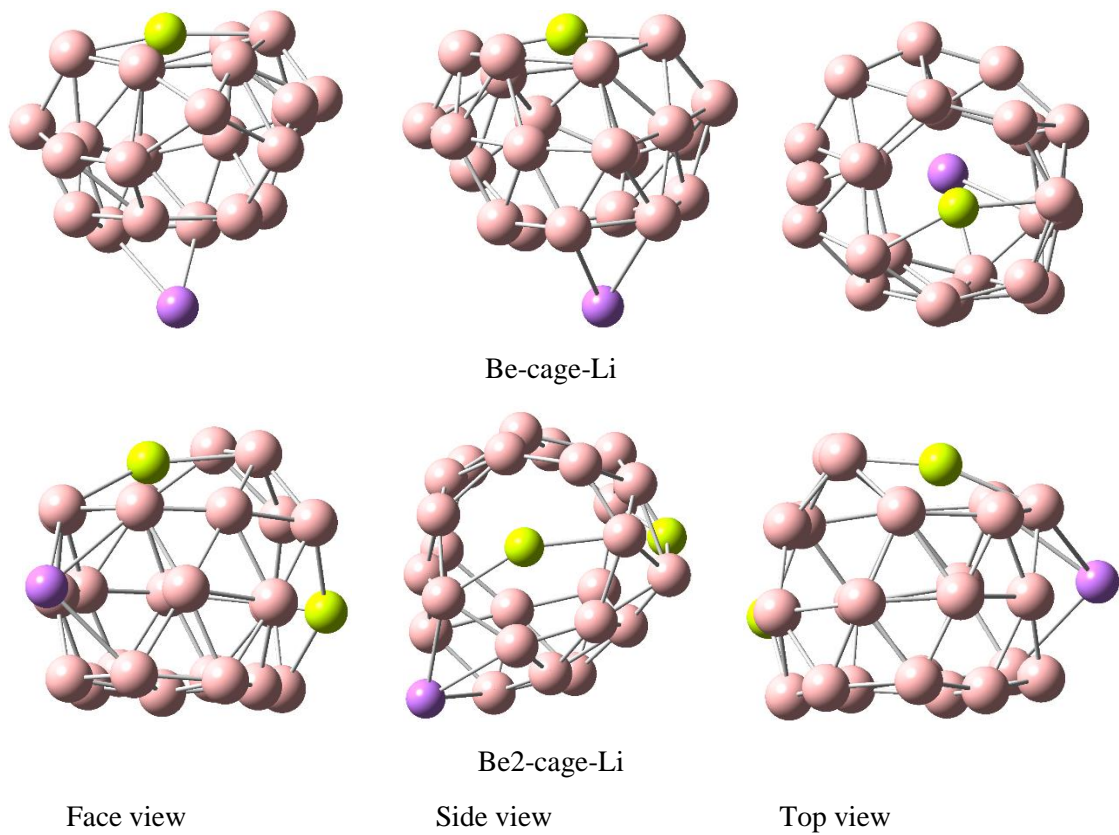


Fig. S1 The optimized geometries for the adsorption of the Be and the Li on the B₂₄.

Table S2. The HOMO-LUMO energy gap and the HOMO and the LUMO energies in eV.

Species	HOMO energy	LUMO energy	HOMO-LUMO energy gap
ring	-6.08	-3.98	2.10
Be-ring	-5.81	-4.02	1.79
2Be-ring	-5.70	-3.28	2.24
tube	-5.88	-3.74	2.14
Be-tube	-5.83	-3.48	2.35
2Be-tube	-5.30	-3.41	1.89
convex	-6.26	-4.47	1.79
Be-convex	-6.28	-4.29	1.99
2Be-convex	-6.14	-3.89	2.25
quasiplanar	-6.33	-4.25	2.08
Be-quasiplanar	-6.23	-4.36	1.87
2Be-quasiplanar	-6.04	-4.24	1.80
cage	-5.48	-3.54	1.94
Be-cage	-6.12	-3.31	2.81
2Be-cage	-6.10	-3.31	2.79

Table S3. The NBO charges of the nBe@B₂₄ (n = 1 and 2) molecules.

Atoms	Species									
	Be-ring	2Be-ring	Be-tube	2Be-tube	Be-convex	2Be-convex	Be-quasi planar	2Be-quasi planar	Be-cage	2Be-cage
B1	0.14	0.14	-0.03	-0.05	0.06	-0.28	0.09	0.11	-0.12	-0.13
B2	0.14	0.14	-0.15	-0.15	0.06	0.02	-0.15	-0.31	-0.07	-0.06
B3	-0.01	0.00	-0.28	-0.29	-0.04	0.02	-0.08	-0.08	-0.28	-0.19
B4	0.05	0.11	-0.03	-0.05	0.08	0.12	-0.12	-0.20	0.47	0.36
B5	-0.09	-0.14	-0.15	-0.15	-0.07	-0.10	0.12	-0.11	-0.03	-0.11
B6	0.060	0.11	-0.28	-0.29	0.10	0.13	-0.05	-0.02	-0.19	-0.06
B7	-0.01	0.00	-0.01	-0.09	-0.19	-0.27	0.28	0.15	0.11	-0.10
B8	-0.01	0.14	-0.01	-0.09	-0.07	0.03	0.03	0.04	-0.01	0.14
B9	0.060	0.14	-0.06	0.01	-0.31	-0.35	-0.22	-0.37	0.01	-0.06
B10	-0.09	-0.09	0.24	0.22	-0.03	-0.12	0.06	0.10	-0.01	-0.01
B11	0.05	0.13	0.00	0.03	0.10	0.34	0.13	0.16	-0.33	0.03
B12	-0.01	-0.09	-0.06	0.01	-0.20	0.02	0.00	0.09	-0.07	-0.06
B13	-0.19	-0.24	0.24	0.22	0.03	-0.18	-0.15	-0.10	0.21	-0.18
B14	-0.24	-0.22	0.00	0.03	0.04	-0.19	-0.13	-0.10	-0.08	0.13
B15	-0.19	-0.22	-0.05	-0.07	-0.04	-0.32	-0.04	0.08	0.31	-0.15
B16	-0.33	-0.35	-0.05	-0.07	0.02	0.01	0.17	0.05	-0.30	-0.20
B17	0.05	0.00	0.18	-0.04	0.02	-0.21	-0.33	-0.40	0.09	-0.28
B18	-0.05	0.00	-0.15	-0.26	-0.11	-0.36	-0.15	-0.04	-0.21	-0.21
B19	0.02	-0.35	-0.01	-0.10	-0.09	-0.17	-0.07	-0.40	0.01	0.15
B20	-0.04	-0.22	0.18	-0.04	-0.11	-0.09	-0.21	-0.19	-0.10	-0.22
B21	0.02	-0.22	-0.15	-0.26	-0.08	-0.04	-0.23	-0.18	-0.05	-0.14
B22	-0.05	-0.24	-0.01	-0.10	-0.03	-0.04	-0.07	-0.21	-0.07	0.09
B23	0.05	-0.25	-0.07	-0.03	0.08	0.28	0.04	0.02	-0.04	0.05
B24	-0.33	-0.25	-0.07	-0.03	-0.13	0.10	0.33	0.32	-0.06	-0.13
Be1	0.96	0.97	0.79	0.86	0.87	0.76	0.72	0.69	0.79	0.73
Be2	-----	0.97	-----	0.77	-----	0.88	-----	0.90	-----	0.60

Table S4. The interatomic distance (\AA) and the values of the electron density ($\rho(r)$) and $\nabla^2\rho(r)$ (in a.u.) in the Be-B and the Be-Be interactions.

Species	Interaction	Interatomic distance	$\rho(r)$	$\nabla^2\rho(r)$
Be-ring	Be1-B16	2.00	0.06	0.11
	Be1-B24	2.00	0.06	0.11
2Be-ring	Be1-B13	1.87	0.06	0.12
	Be1-B16	1.97	0.06	0.11
	Be2-B19	1.87	0.06	0.11
Be-tube	Be2-B22	1.97	0.06	0.12
	Be1-B7	1.84	0.08	0.16
	Be1-B8	1.84	0.08	0.16
2Be-tube	Be1-B7	1.91	0.07	0.15
	Be1-B8	1.91	0.07	0.15
	Be2-B17	1.87	0.07	0.16
	Be2-B20	1.87	0.07	0.16
Be-convex	Be1-B7	1.90	0.06	0.12
	Be1-B9	1.79	0.08	0.17
	Be1-B12	1.90	0.06	0.12
2Be-convex	Be1-B9	1.85	0.07	0.18
	Be1-B12	1.86	0.06	0.14
	Be2-B13	1.87	0.07	0.16
	Be2-B18	1.90	0.08	0.14
Be-quasiplanar	Be1-B18	1.80	0.07	0.18
	Be1-B21	1.84	0.07	0.17
2Be-quasiplanar	Be1-B20	1.86	0.07	0.17
	Be2-B22	1.89	0.06	0.17
Be-cage	Be1-B3	1.86	0.07	0.15
	Be1-B18	1.88	0.07	0.16
2Be-cage	Be1-B3	1.86	0.07	0.15
	Be1-B18	1.88	0.07	0.16
	Be2-B15	1.77	0.07	0.17
	Be2-B17	1.81	0.07	0.18

Table S5. The values of the total first hyperpolarizability, β_{total} , and its corresponding components (in a.u.) for all the reported the $n\text{Be}@B_{24}$ ($n = 1$ and 2) molecules.

Components	Species									
	Be-ring	2Be-ring	Be-tube	2Be-tube	Be-convex	2Be-convex	Be-quasiplanar	2Be-quasiplanar	Be-cage	2Be-cage
β_{total}	558	277	270	44	304	448	810	229	272	351
β_{xxx}	684	53	-1	2	-5	544	-1198	-137	56	23
β_{xyy}	-18	-169	11	120	-457	-270	-115	-120	-123	-243
β_{xyy}	185	21	-8	2	-7	209	-164	-197	-25	140
β_{yyy}	-37	41	24	-86	-24	193	346	70	-22	-219
β_{xxz}	-98	202	53	-10	-59	68	-82	-182	-86	-79
β_{yyz}	56	-9	53	-15	-201	-21	-19	-55	203	-92
β_{xzz}	50	16	7	10	-2	-54	115	29	-93	138
β_{yzz}	-6	-7	5	-76	114	323	78	-49	14	-28
β_{zzz}	-89	223	341	-35	-90	54	518	443	313	283
β_x	551	53	-2	8	-8	419	-748	-183	-37	180
β_y	-36	-81	24	-25	-220	147	186	-59	-78	-294
β_z	-79	260	269	-36	-210	60	251	124	258	67