Electronic Supplementary Material (ESI) for Dalton Transactions.

Mixed superalkalis are better choice than pure superalkalis for $B_{12}N_{12}$ nanocage to design high performance nonlinear optical materials

Rehana Bano[a], Khurshid Ayub[b], Tariq Mahmood[b,c], Muhammad Arshad[d], Ahsan Sharif[a], Sobia Tabassum[e] , Mazhar Amjad Gilani[f]*

[a]*School of Chemistry, University of the Punjab, Lahore-54590, Pakistan*

[b]*Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, Abbottabad-22060, Pakistan*

[c]Department of Chemistry, College of Science, University of Bahrain, P.O. Box 32038, Bahrain

[d]*Institute of Chemistry, The Islamia University of the Bahawalpur, Bahawalpur-63100, Pakistan*

[e]*Interdisciplinary Research Centre in Biomedical Materials (IRCBM), COMSATS University Islamabad, Lahore Campus, Lahore-54600, Pakistan*

[f]*Department of Chemistry, COMSATS University Islamabad, Lahore Campus, Lahore-54600, Pakistan*

***Corresponding Author**

E-mail Address: **mazhargilani@cuilahore.edu.pk**

(M.A. Gilani)

Supplementary Information

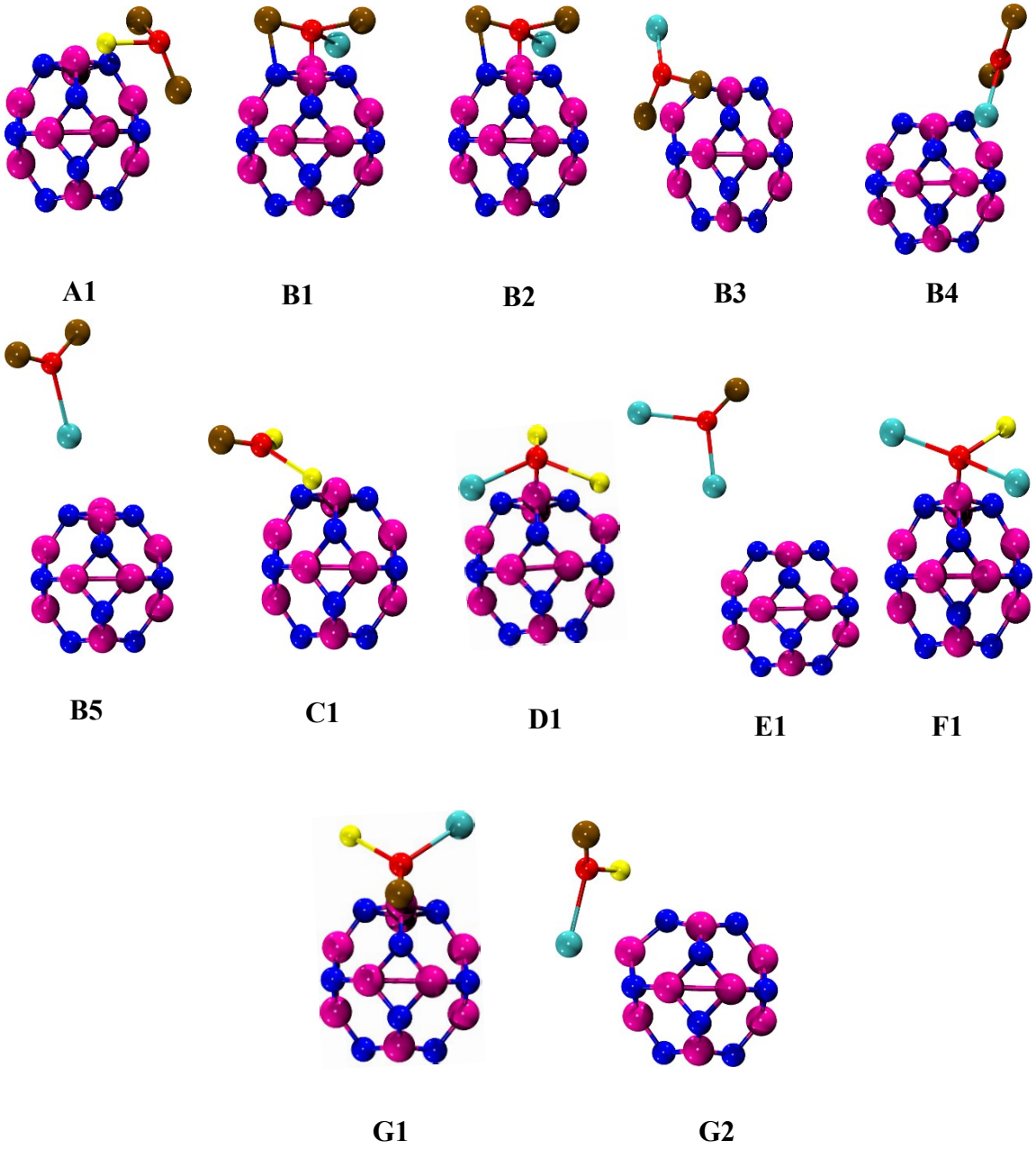
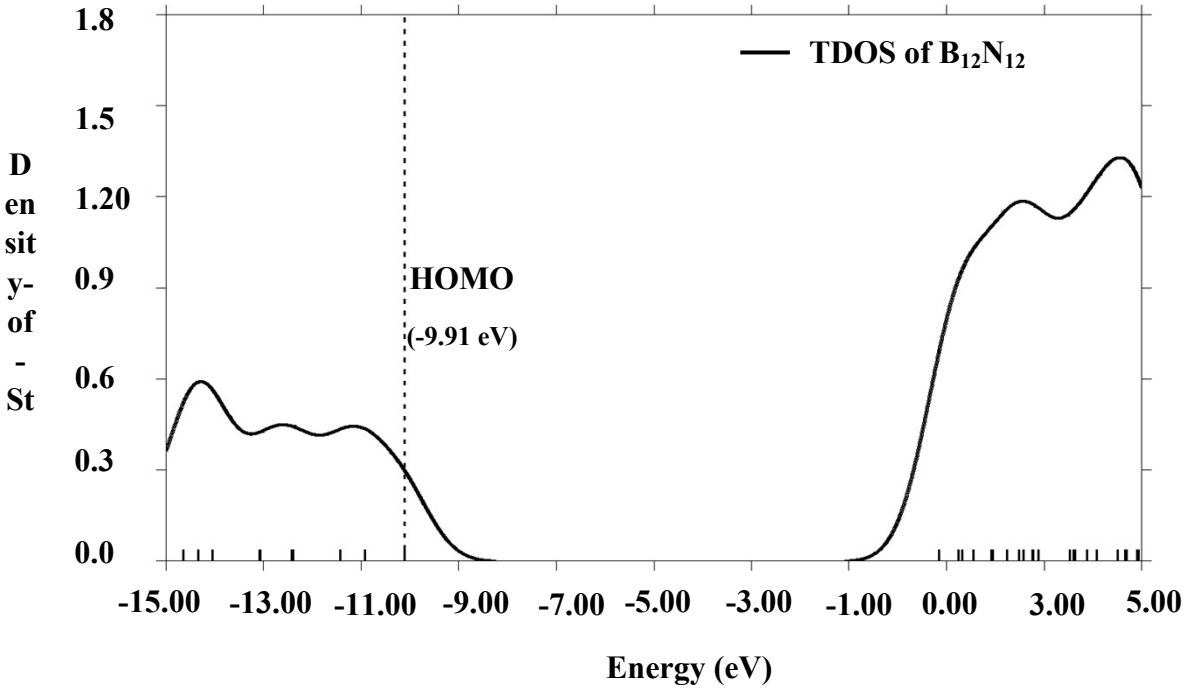
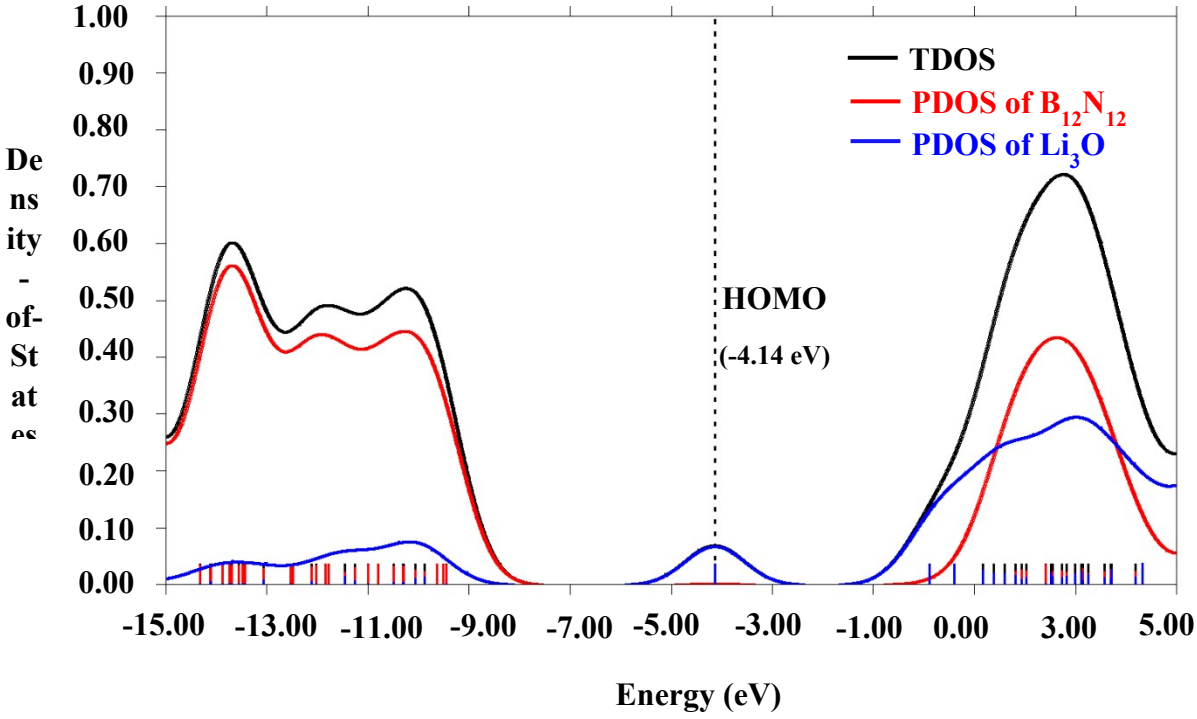
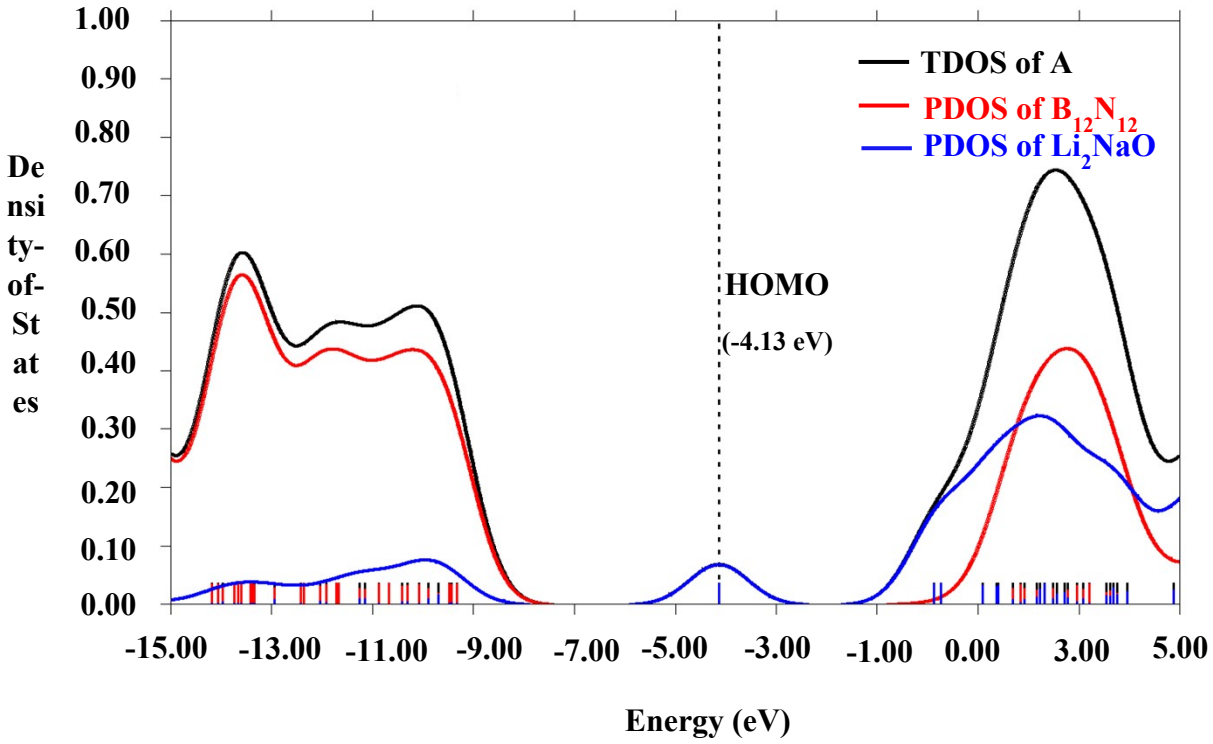
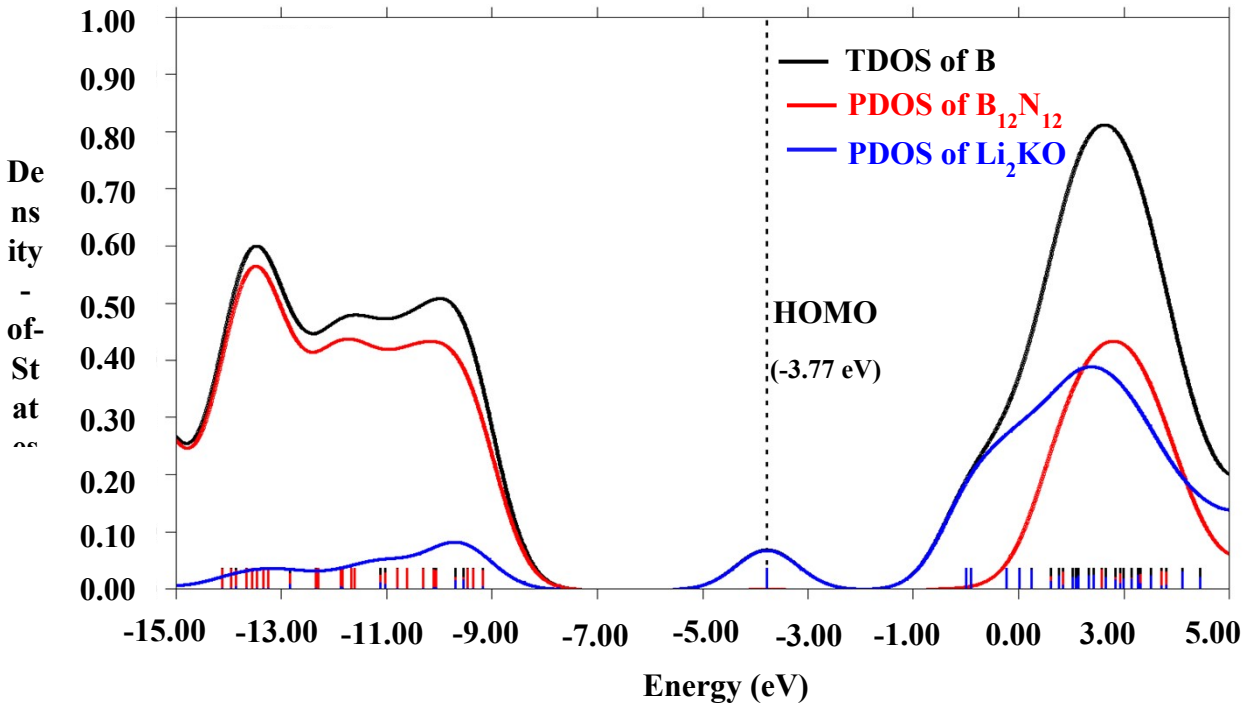


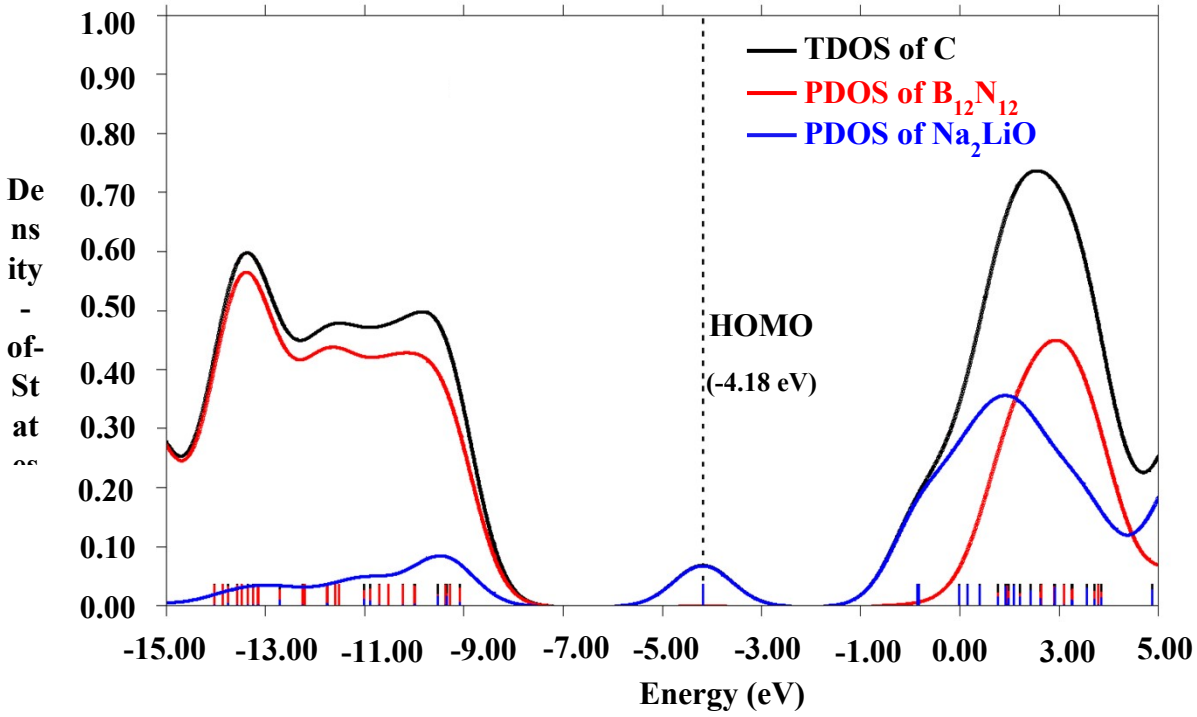
Fig. S1: Optimized geometries of other isomers of **A-G** complexes (other than most stable complexes)

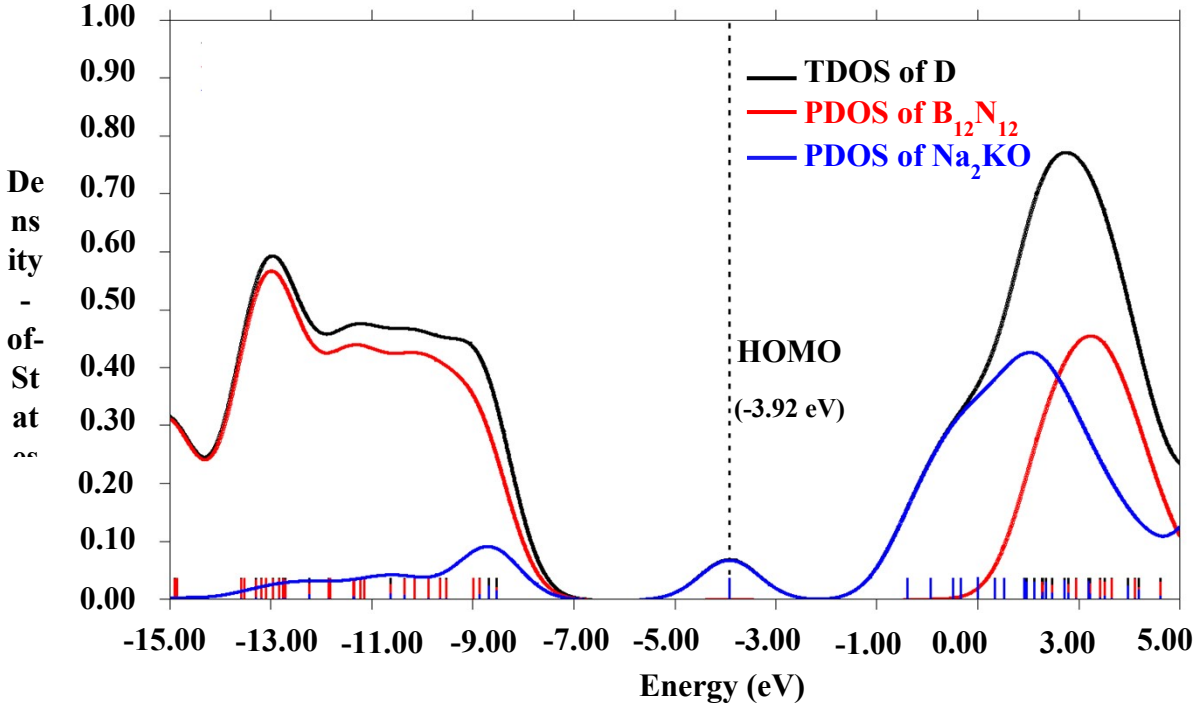

TDOS of $B_{12}N_{12}$
HOMO
(-9.91 eV)
Density-of-States
Energy (eV)

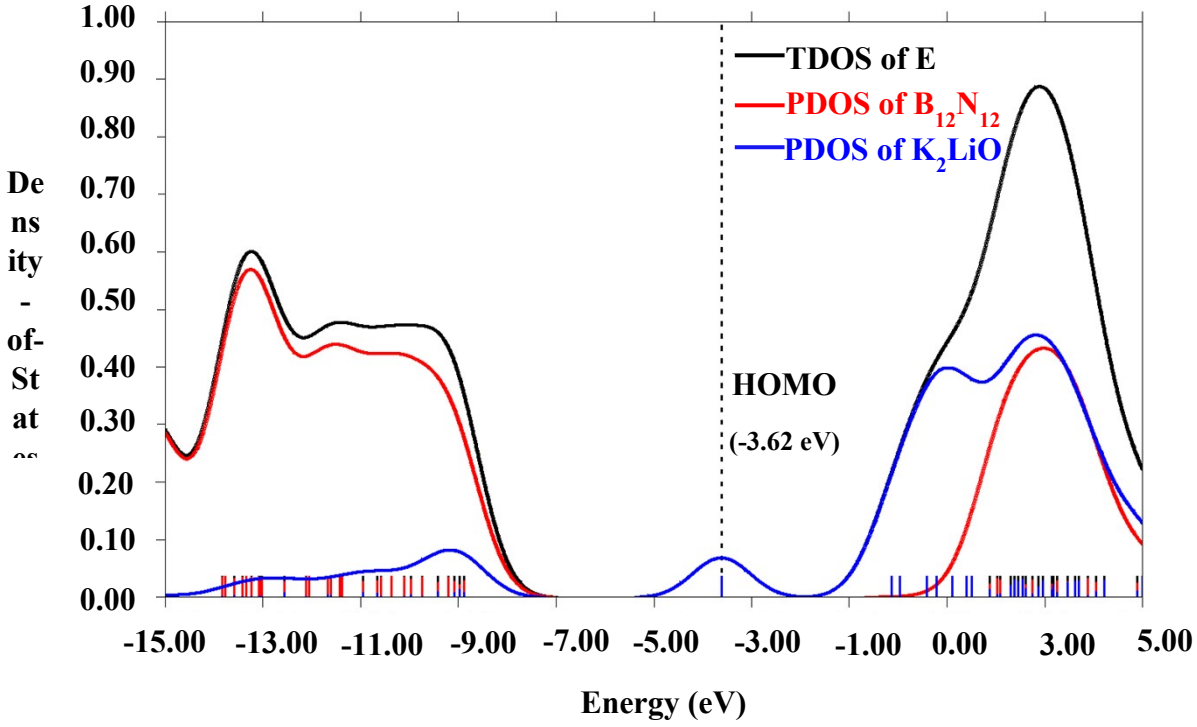

TDOS
PDOS of $B_{12}N_{12}$
PDOS of Li_3O
HOMO
(-4.14 eV)
Density-of-States
Energy (eV)

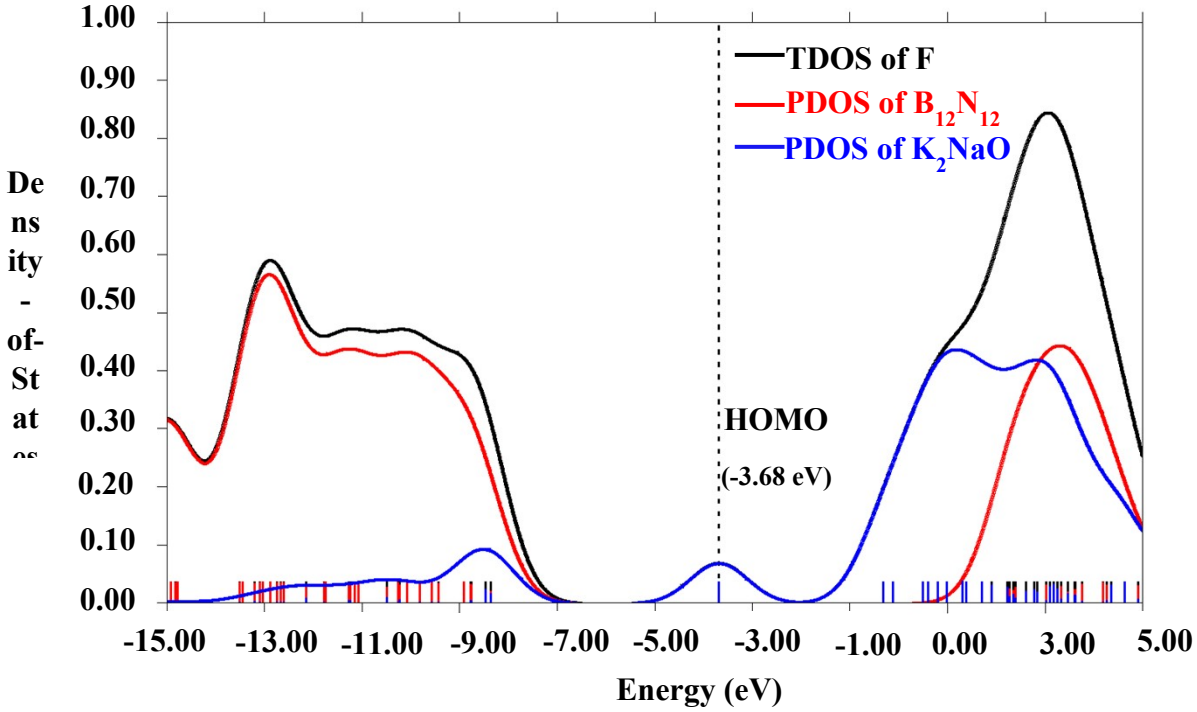

Density-of-States
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
TDOS of A
PDOS of B12N12
PDOS of Li2NaO
HOMO
(-4.13 eV)
-15.00
-13.00
-11.00
-9.00
-7.00
-5.00
-3.00
-1.00
0.00
3.00
5.00
Energy (eV)


Density-of-States
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
TDOS of B
PDOS of B12N12
PDOS of Li2KO
HOMO
(-3.77 eV)
-15.00
-13.00
-11.00
-9.00
-7.00
-5.00
-3.00
-1.00
0.00
3.00
5.00
Energy (eV)


TDOS of C
PDOS of $B_{12}N_{12}$
PDOS of Na_2LiO
HOMO
(-4.18 eV)
Density-of-States
Energy (eV)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
-15.00
-13.00
-11.00
-9.00
-7.00
-5.00
-3.00
-1.00
0.00
3.00
5.00


TDOS of D
PDOS of $B_{12}N_{12}$
PDOS of Na_2KO
HOMO
(-3.92 eV)
Density-of-States
Energy (eV)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
-15.00
-13.00
-11.00
-9.00
-7.00
-5.00
-3.00
-1.00
0.00
3.00
5.00


TDOS of E
PDOS of B12N12
PDOS of K2LiO
HOMO
(-3.62 eV)
Density-of-States
Energy (eV)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
-15.00
-13.00
-11.00
-9.00
-7.00
-5.00
-3.00
-1.00
0.00
3.00
5.00


TDOS of F
PDOS of B12N12
PDOS of K2NaO
HOMO
(-3.68 eV)
Density-of-States
Energy (eV)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
-15.00
-13.00
-11.00
-9.00
-7.00
-5.00
-3.00
-1.00
0.00
3.00
5.00

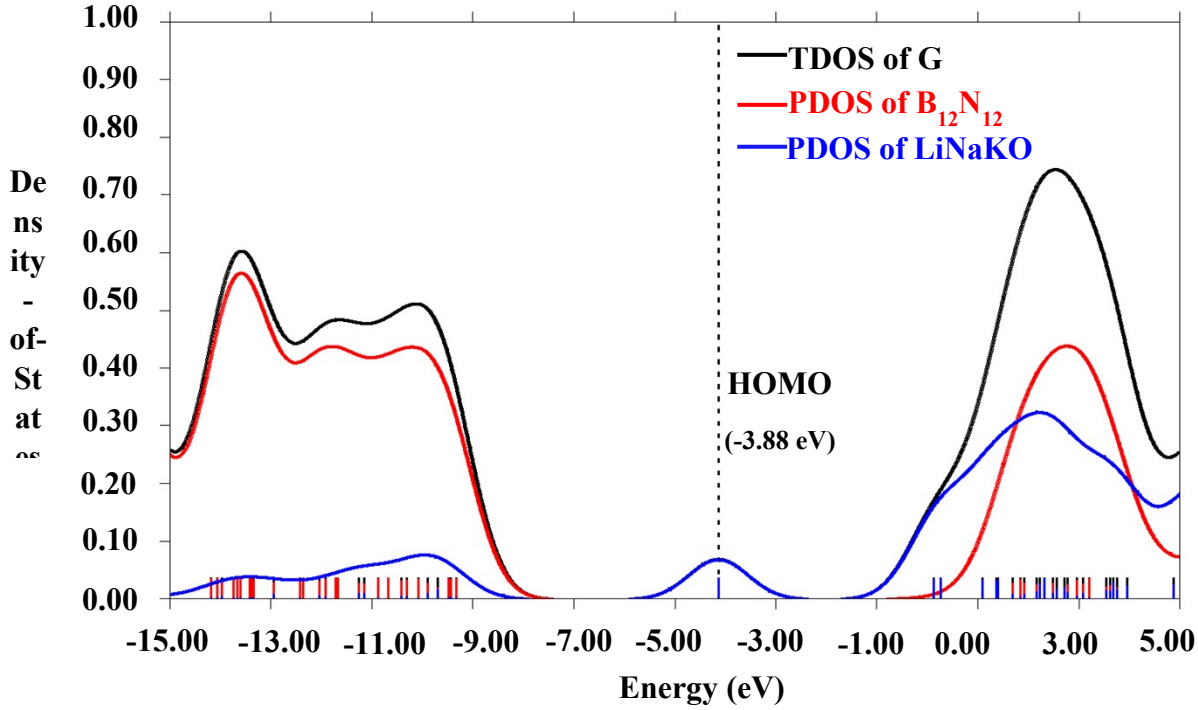


Fig. S2. TDOS and PDOS spectra of $B_{12}N_{12}$ and mixed superalkali doped $B_{12}N_{12}$ complexes

Table S1: The AIM topological parameters, including electron density (ρ), Laplacian of electron density ($\nabla^2\rho$), electron energy density H(r) and the ratio of the kinetic electron density G(r) to potential electron density V(r) at BCPs of the doped isomers (All the values are in au)

Isomer	Interaction	ρ	$\nabla^2\rho$	G(r)	V(r)	H(r)	-G(r)/V(r)
A	Li-N	0.0206	0.1306	0.0274	-0.0221	0.0053	1.2398
	Li-N	0.0293	0.1899	0.0407	-0.0339	0.0067	1.2006
	O-B	0.1971	0.5721	0.3309	-0.5187	-0.1878	0.6379
B	Li-N	0.0201	0.1267	0.0265	-0.0213	0.0052	1.2441
	Li-N	0.0289	0.1877	0.0402	-0.0335	0.0067	1.2000
	K-N	0.0132	0.0536	0.0111	-0.0086	0.0023	1.2907
	O-B	0.1996	0.5822	0.3371	-0.5286	-0.1915	0.6377
C	Li-N	0.0295	0.1925	0.0413	-0.0344	0.0069	1.2006
	Na-N	0.0156	0.0849	0.0174	-0.0138	0.0037	1.2609
	Na-N	0.0156	0.0848	0.0174	-0.0138	0.0037	1.2609
	O-B	0.2017	0.5861	0.3412	-0.5361	-0.1947	0.6364
D	Na-N	0.0172	0.0948	0.0195	-0.0155	0.0042	1.2581
	Na-N	0.0172	0.0948	0.0195	-0.0155	0.0042	1.2581
	K-N	0.0196	0.0842	0.0177	-0.0144	0.0033	1.2292
	O-B	0.2101	0.6265	0.3629	-0.5693	-0.2063	0.6374
E	Li-N	0.0312	0.2039	0.0439	-0.0368	0.0071	1.1929
	K-N	0.0141	0.0585	0.0121	-0.0095	0.0026	1.2737
	K-N	0.0145	0.0602	0.0124	-0.0097	0.0026	1.2784

	O-B	0.2078	0.6193	0.3579	-0.5611	-0.2031	0.6379
F	Na-N	0.0162	0.0894	0.0184	-0.0145	0.0039	1.2690
	K-N	0.0172	0.0731	0.0153	-0.0121	0.0031	1.2645
	K-N	0.0189	0.0811	0.0169	-0.0137	0.0031	1.2336
	O-B	0.2127	0.6414	0.3703	-0.5803	-0.2099	0.6381
G	Li-N	0.0307	0.1999	0.0429	-0.0359	0.0069	1.1950
	Na-N	0.0136	0.0726	0.0149	-0.0117	0.0032	1.2735
	K-N	0.0147	0.0613	0.0126	-0.0099	0.0027	1.2727
	O-B	0.2048	0.6031	0.3496	-0.5485	-0.1988	0.6374