Supporting Information for

Computational mining of endohedral C_{70} electrides: Tri-metal alkalis and alkaline-earth encapsulation

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Table S1. Relative energies ΔE (kcal·mol^{-1}) of $Li_3@C_{70}$ and $Be_3@C_{70}$ isomers at the M06-2X/def2-TZVP level

Spiral number	Symmetry	Pentagon adjacencies	ΔE $Li_3@C_{70}$	ΔE $Be_3@C_{70}$
8149	D_{5h}	0	0.00	0.00
8144	C_s	2	19.69	31.95
8094	C_s	1	41.54	11.20
7957	C_2	2	27.54	45.37
7922	C_s	3	60.77	53.92
7921	C_1	3	40.49	45.28
7893	C_1	3	32.62	39.01
7892	C_2	2	3.63	7.53
7887	C_2	3	35.88	42.98
7886	C_1	3	41.31	48.48
7854	C_{2v}	3	33.99	39.38
7852	C_1	3	43.85	43.40
7851	C_1	3	31.44	47.86
7850	C_2	3	49.66	54.59
7849	C_1	3	33.87	36.33
7848	C_1	3	53.66	59.98

Table S2. The relaxed M-M distances $d_{M\text{-}M}$ (Å) of M_3 (M = Li, Na, K, Be, Mg, Ca, Sr and Ba) clusters in free state

Systems	$d_{M1\text{-}M2}$	$d_{M2\text{-}M3}$	$d_{M1\text{-}M3}$
Li_3	3.38	2.79	2.79
Na_3	3.22	3.22	4.78
K_3	4.17	6.29	4.17
Be_3	2.17	2.17	2.17
Mg_3	3.48	3.48	3.48
Ca_3	4.32	4.32	4.32
Sr_3	5.23	5.21	5.24
Ba_3	5.79	5.79	5.79

Table S3. Natural population analysis (NPA) charges (e) and natural electron configuration populations for metal atoms in $M_3@C_{70}$

Isomers	NPA Charge	Natural electron configuration populations
$Li_3@C_{70}$	0.58/0.62/0.62	Li1: $2s^{0.34}2p^{0.07}3s^{0.01}$
		Li2: $2s^{0.31}2p^{0.06}3s^{0.01}$
		Li3: $2s^{0.31}2p^{0.06}3s^{0.01}$
$Na_3@C_{70}$	0.62/0.57/0.68	Na1: $3s^{0.34}3p^{0.02}4s^{0.01}3d^{0.01}$
		Na2: $3s^{0.39}3p^{0.02}4s^{0.01}$
		Na3: $3s^{0.28}3p^{0.02}4s^{0.01}3d^{0.01}$
$K_3@C_{70}$	0.90/0.91/0.90	K1: $4s^{0.12}3d^{0.02}4d^{0.01}$
		K2: $4s^{0.12}3d^{0.02}4d^{0.01}$
		K3: $4s^{0.12}3d^{0.02}4d^{0.01}$
$Be_3@C_{70}$	0.67/0.56/0.67	Be1: $2s^{1.19}2p^{0.13}3d^{0.01}$
		Be2: $2s^{1.25}2p^{0.19}3d^{0.01}$
		Be3: $2s^{1.19}2p^{0.13}3d^{0.01}$
$Mg_3@C_{70}$	1.35/1.17/1.35	Mg1: $3s^{0.56}3p^{0.04}3d^{0.04}$
		Mg2: $3s^{0.73}3p^{0.06}3d^{0.04}$
		Mg3: $3s^{0.56}3p^{0.04}3d^{0.04}$
$Ca_3@C_{70}$	1.16/1.25/1.27	Ca1: $4s^{0.62}3d^{0.16}4p^{0.01}5s^{0.01}4d^{0.01}5p^{0.04}$
		Ca2: $4s^{0.56}3d^{0.13}5s^{0.01}4d^{0.01}5p^{0.04}$
		Ca3: $4s^{0.50}3d^{0.17}5s^{0.01}4d^{0.01}5p^{0.04}$
$Sr_3@C_{70}$	1.56/1.56/1.55	Sr1: $5s^{0.36}6s^{0.01}6p^{0.10}$
		Sr2: $5s^{0.36}6s^{0.01}6p^{0.10}$
		Sr3: $5s^{0.37}6s^{0.01}6p^{0.11}$
$Ba_3@C_{70}$	1.89/1.89/1.89	Ba1: $6s^{0.13}6p^{0.02}7p^{0.02}$
		Ba2: $6s^{0.13}6p^{0.02}7p^{0.02}$
		Ba3: $6s^{0.12}6p^{0.01}7p^{0.03}$

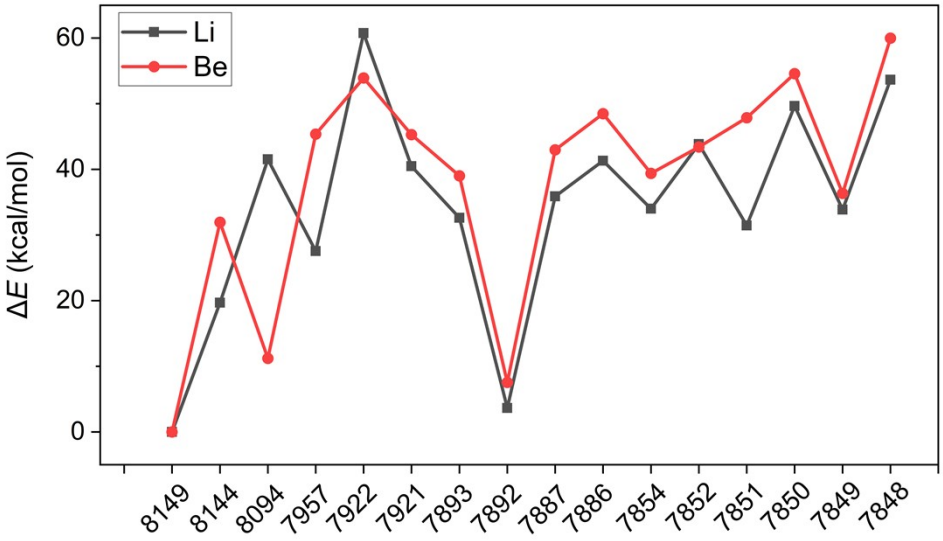

Figure S1. Relative energies of different $Li_3@C_{70}$ and $Be_3@C_{70}$ isomers.

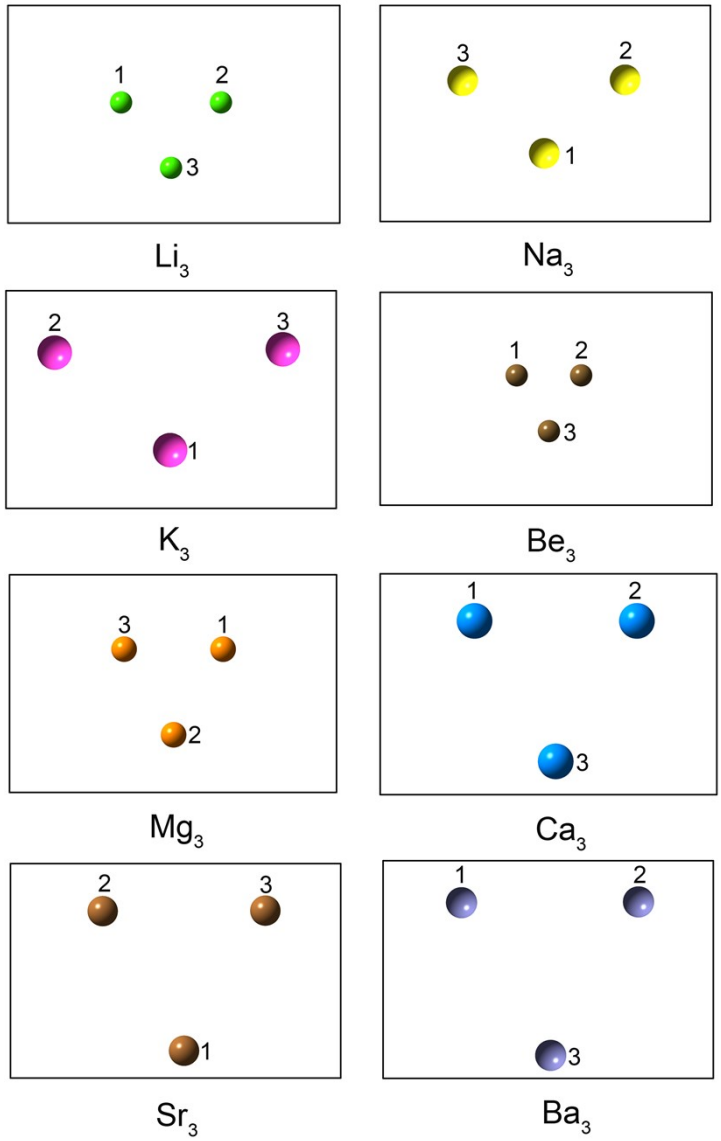

Figure S2. The optimized geometries of M_3 (M = Li, Na, K, Be, Mg, Ca, Sr and Ba). Li, Na, K, Be, Mg, Ca, Sr and Ba atoms are marked with green, yellow, mauve, ochre, orange, blue, pink and ice blue color, respectively.

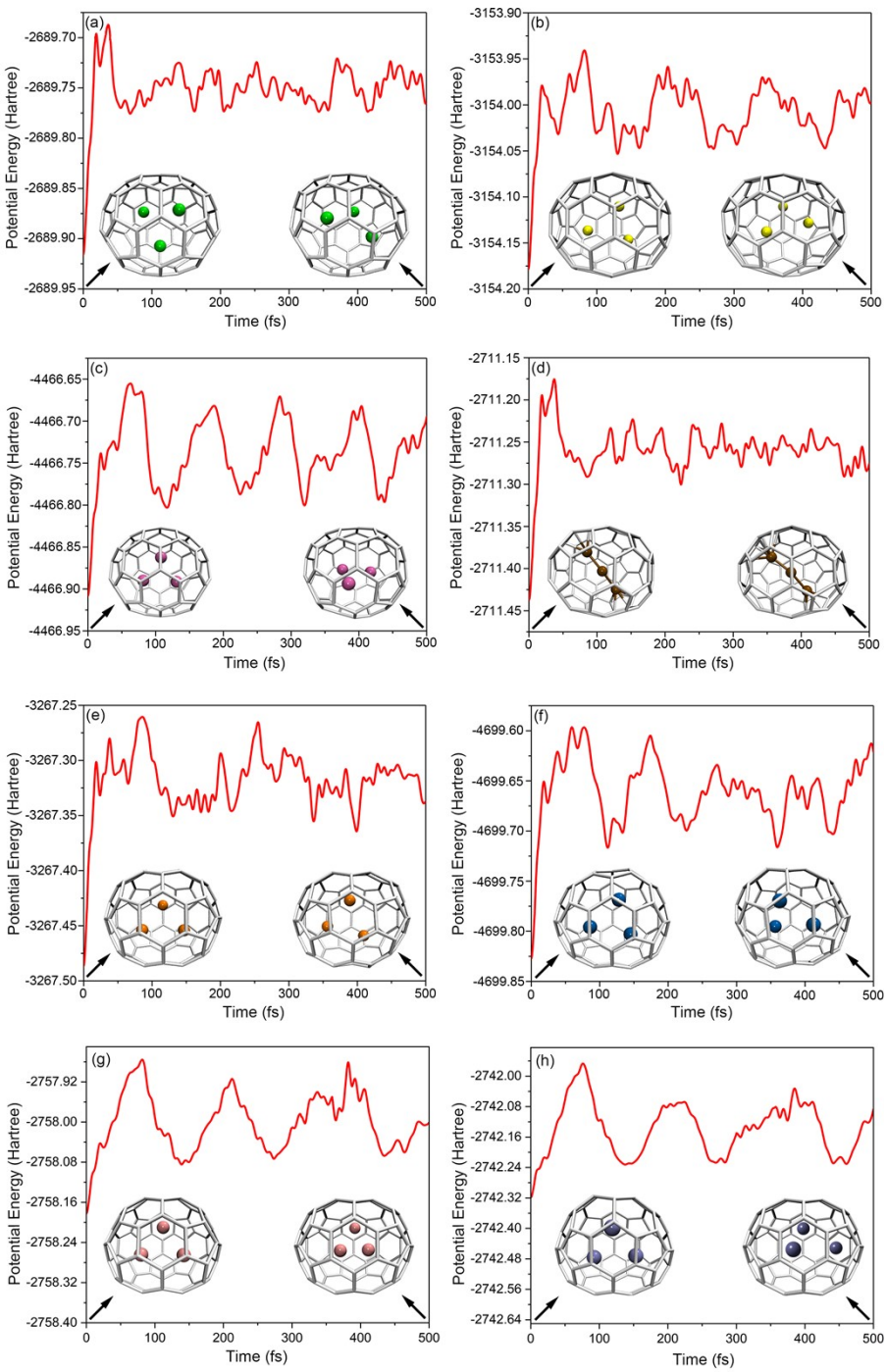

Figure S3. Plots of potential energy versus the time of trajectory of (a) $Li_3@C_{70}$, (b) $Na_3@C_{70}$, (c) $K_3@C_{70}$, (d) $Be_3@C_{70}$, (e) $Mg_3@C_{70}$, (f) $Ca_3@C_{70}$, (g) $Sr_3@C_{70}$, and (h) $Ba_3@C_{70}$ using the ADMP method. The structures at the start and end of trajectory are also depicted.

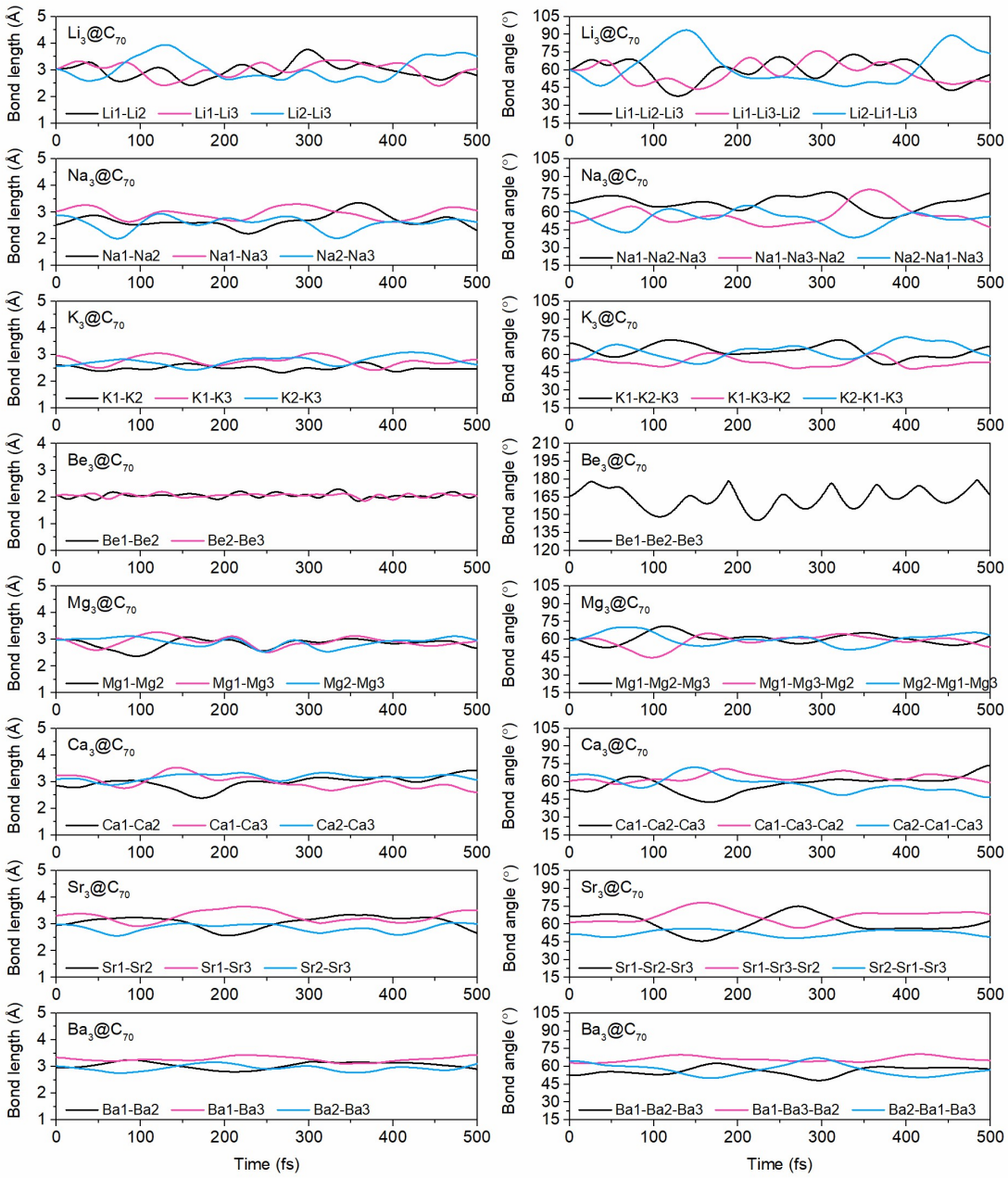

Figure S4. Variations of M-M bond length and M-M-M bond angle versus the time of trajectory for M_3 clusters in $M_3@C_{70}$ using the ADMP method.

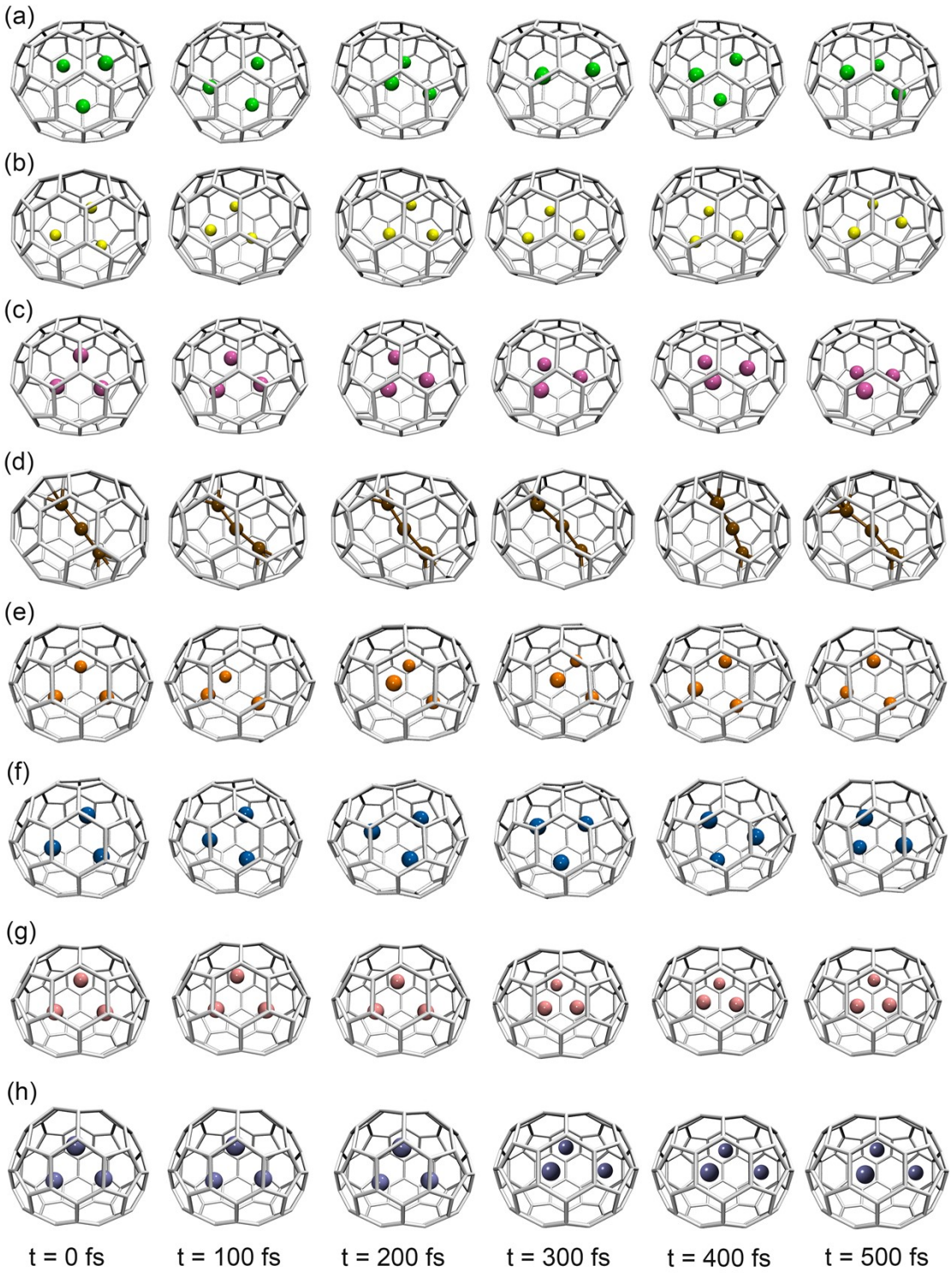

Figure S5. Structure snapshots at different time at 500 K for (a) $Li_3@C_{70}$, (b) $Na_3@C_{70}$, (c) $K_3@C_{70}$, (d) $Be_3@C_{70}$, (e) $Mg_3@C_{70}$, (f) $Ca_3@C_{70}$, (g) $Sr_3@C_{70}$, and (h) $Ba_3@C_{70}$.

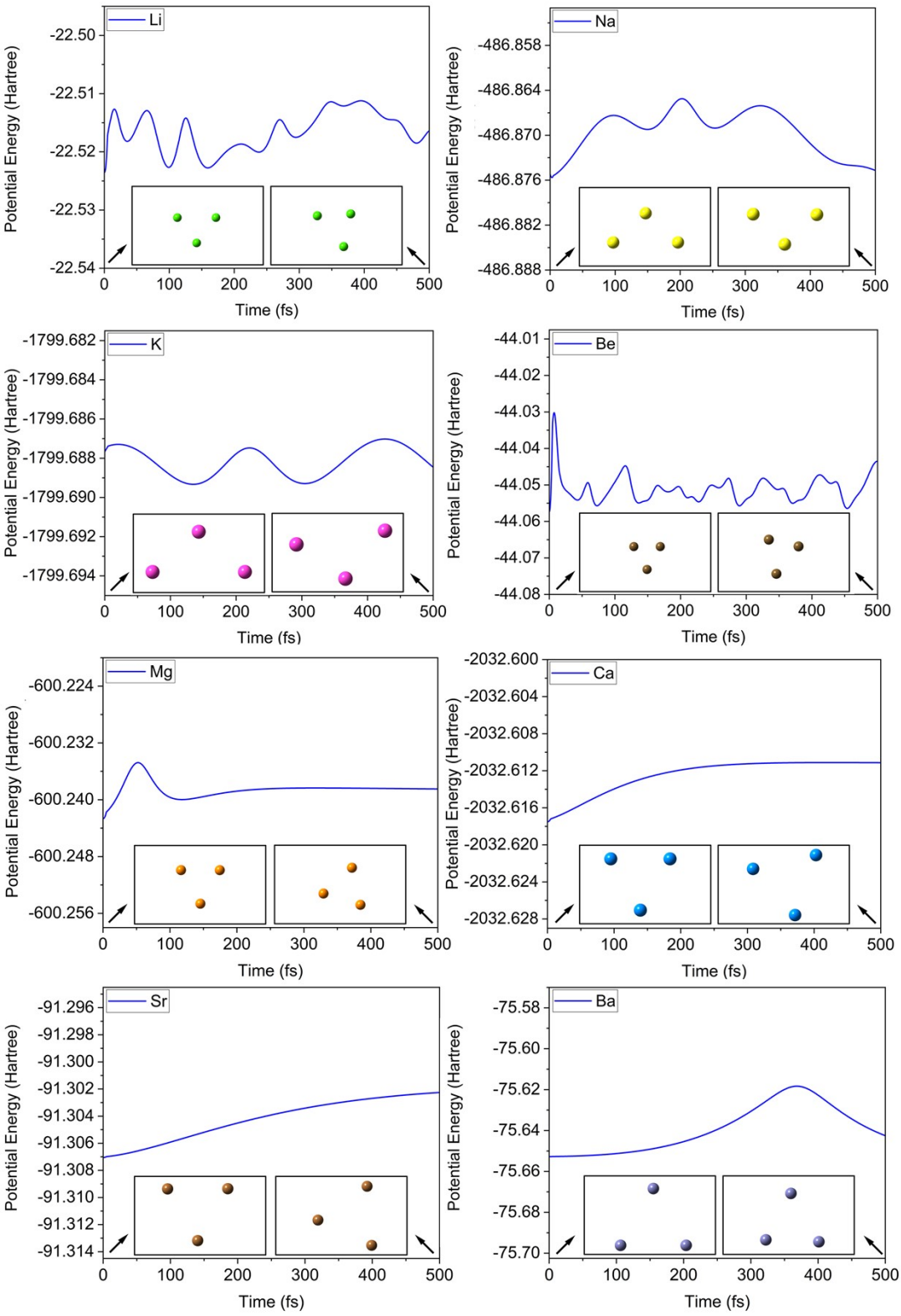

Figure S6. Plots of potential energy versus the time of trajectory of M_3 clusters at 500 K. The structures at the start and end of trajectory are also depicted.

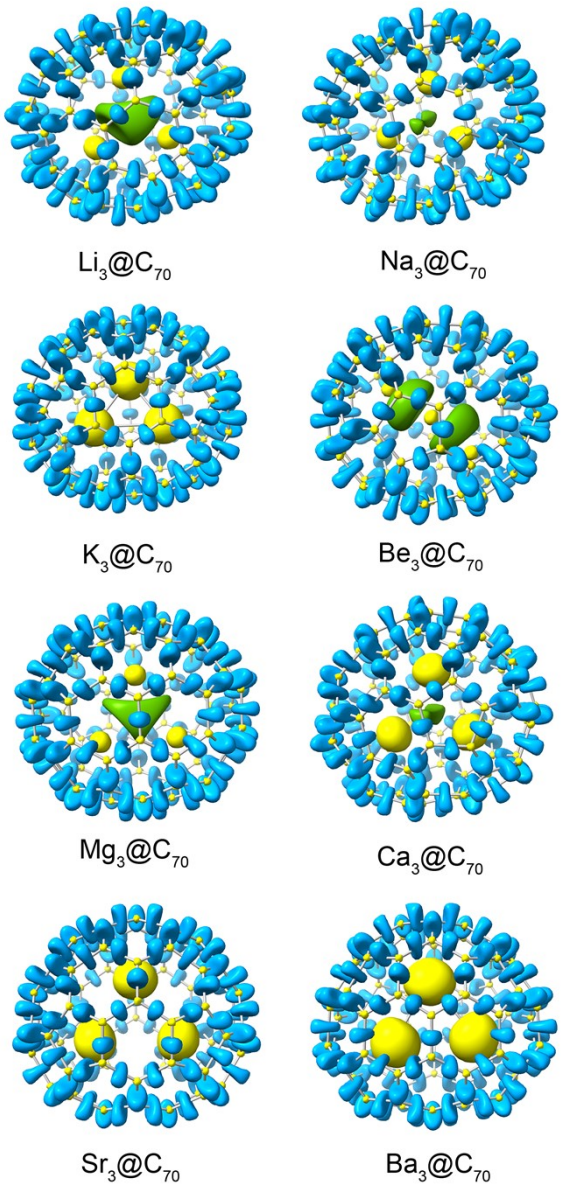

Figure S7. Custom colored 3D isosurface of electron localization function (ELF) maps for $M_3@C_{70}$.