Supporting Materials

Probing the structural evolution, electronic and spectral properties of beryllium doped magnesium and their ions clusters

Lu Zeng,* Mei-Kun Liang, Xiao-Fan Wei, Jia Guo, Shuai Zhang, Jie Bi, Wei Dai* and Ben-Chao Zhu*

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Table S1. Electronic State, symmetries, E_b , $\Delta_2 E$, E_{gap} and charges on Be atoms in the ground state of $BeMg_n^Q$ (Q = 0, ±1; n = 2 – 12) clusters at PBE0 / 6-311G(d, p) level.

n	Anionic $BeMg_n^{Q=-1}$							Neutral $BeMg_n^{Q=0}$						Cationic $BeMg_n^{Q=+1}$						
	Symm	State	E_b (eV)	$\Delta_2 E$ (eV)	αEgap (eV)	βEgap (eV)	Charges on Be (e)	Symm	State	E_b (eV)	$\Delta_2 E$ (eV)	αEgap (eV)	Charges on Be (e)	Symm	State	E_b (eV)	$\Delta_2 E$ (eV)	αEgap (eV)	βEgap (eV)	Charges on Be (e)
2	$C_{\infty V}$	$^2A_1$	0.59	—	1.21	2.01	-0.87	C_{2V}	$^1A_1$	0.25	—	2.85	-0.30	C_{3V}	$^2A_1$	0.60	—	1.70	3.96	-0.34
3	C_{3V}	$^2A_1$	0.88	1.13	1.70	2.81	-0.97	C_{3V}	$^1A_1$	0.50	0.75	2.86	-0.72	C_{3V}	$^2A_1$	0.88	0.47	3.29	1.66	-1.26
4	C_{3V}	$^2A_1$	0.83	-0.01	1.54	2.27	-1.69	C_{3V}	$^1A_1$	0.50	-0.10	2.12	-1.63	C_S	$^2A'$	0.96	0.56	2.17	2.78	-1.66
5	C_2	^2B	0.79	-0.50	1.92	1.84	-1.76	C_{2V}	$^1A_1$	0.51	-0.28	1.89	-1.97	C_1	^2A	0.92	-0.02	1.78	2.73	-1.52
6	C_S	$^2A'$	0.84	0.12	1.24	2.20	-2.14	C_S	$^1A'$	0.57	0.18	2.16	-1.77	C_S	$^2A'$	0.89	-0.16	1.75	2.02	-2.43
7	C_1	^2A	0.86	-0.51	1.44	2.00	-2.67	C_S	$^1A'$	0.58	-0.62	1.89	-2.32	C_1	^2A	0.89	-0.16	1.75	2.10	-2.25
8	C_S	$^2A'$	0.93	0.28	2.03	1.73	-1.52	C_S	$^1A'$	0.67	-0.36	1.93	-1.54	C_1	^2A	0.91	-0.50	1.77	1.88	-2.24
9	C_1	$_2A$	0.96	0.35	1.26	2.28	-2.83	C_S	$^1A'$	0.77	1.24	2.31	-2.74	C_S	$^2A'$	0.98	0.82	2.26	1.69	-2.07
10	C_2	^2B	0.96	0.06	1.15	1.49	-2.99	C_1	^1A	0.74	-0.45	1.77	-2.88	C_{2V}	$^2B_2$	0.96	-0.21	1.36	2.28	-2.92
11	C_S	$^2A''$	0.95	0.35	1.52	1.34	-3.03	C_S	$^1A'$	0.75	0.30	1.70	-2.92	C_S	$^2A'$	0.96	0.10	1.47	2.35	-2.99
12	C_S	$^2A'$	0.91	—	1.39	1.41	-2.61	C_S	$^1A'$	0.74	—	1.77	-1.96	C_1	^2A	0.95	—	1.58	1.73	-3.02

Table S2. Atoms' coordinate in the most stable $BeMg_8^-$, $BeMg_9$, $BeMg_9^+$ clusters.

B3PW91/6-311G(d, p)				PBE0/6-311G(d, p)			
$BeMg_8^-$	X	Y	Z	$BeMg_8^-$	X	Y	Z
Be1	1.35737300	1.12427500	0.00000000	Be1	1.35679300	1.12155000	0.00000000
Mg2	-0.72941900	1.78056600	1.51289800	Mg2	-0.72750700	1.77061200	1.50978900
Mg3	1.68745500	0.19155100	-2.38609200	Mg3	1.68319400	0.18726900	-2.37995800
Mg4	1.68745500	0.19155100	2.38609200	Mg4	1.68319400	0.18726900	2.37995800
Mg5	-0.72941900	1.78056600	-1.51289800	Mg5	-0.72750700	1.77061200	-1.50978900
Mg6	-0.72941900	-1.43197300	-1.59647800	Mg6	-0.72750700	-1.42055600	-1.58965600
Mg7	1.88290400	-1.60917400	0.00000000	Mg7	1.87648600	-1.60563600	0.00000000
Mg8	-2.79259400	0.15412600	0.00000000	Mg8	-2.78511000	0.15713600	0.00000000
Mg9	-0.72941900	-1.43197300	1.59647800	Mg9	-0.72750700	-1.42055600	1.58965600
$BeMg_9$	X	Y	Z	$BeMg_9$	X	Y	Z
Be1	0.50832000	0.75867000	0.00000000	Be1	-0.50500300	0.75415900	0.00000000
Mg2	-0.51448000	2.25915300	1.68385100	Mg2	-2.27779200	0.38457900	1.67891700
Mg3	-0.51448000	2.25915300	-1.68385100	Mg3	-2.27779200	0.38457900	-1.67891700
Mg4	-0.51448000	-0.76839300	-2.21576400	Mg4	0.51286800	-0.76625800	-2.20814900
Mg5	-1.65175500	-2.46786600	0.00000000	Mg5	1.64603500	-2.45946400	0.00000000
Mg6	2.28476200	0.38550100	1.68424100	Mg6	0.51286800	2.25236900	1.67859900
Mg7	-0.51448000	-0.76839300	2.21576400	Mg7	0.51286800	-0.76625800	2.20814900
Mg8	-2.3566650	0.46421800	0.00000000	Mg8	-1.32242900	-1.99513900	0.00000000
Mg9	2.28476200	0.38550100	-1.68424100	Mg9	0.51286800	2.25236900	-1.67859900
Mg10	1.32737800	-2.00176600	0.00000000	Mg10	2.34883800	0.46183600	0.00000000
$BeMg_9^+$	X	Y	Z	$BeMg_9^+$	X	Y	Z
Be1	-1.70552200	-0.51629200	0.00000000	Be1	-1.66997100	-0.49652000	0.00000000
Mg2	-1.52277500	1.51984100	1.56129100	Mg2	-1.52374700	1.52359900	1.56612900
Mg3	3.00154100	-0.16766500	0.00000000	Mg3	3.00054200	-0.17001400	0.00000000
Mg4	1.03890000	0.06564900	2.25980100	Mg4	1.03111600	0.06591600	2.24976100
Mg5	1.06755600	2.20061100	0.00000000	Mg5	1.06140400	2.17702700	0.00000000
Mg6	1.03890000	0.06564900	-2.25980100	Mg6	1.03111600	0.06591600	-2.24976100
Mg7	-1.52277500	-1.53204400	-2.28719400	Mg7	-1.52374700	-1.52968200	-2.27227800
Mg8	-1.52277500	1.51984100	-1.56129100	Mg8	-1.52374700	1.52359900	-1.56612900
Mg9	0.51270900	-1.96774000	0.00000000	Mg9	0.52746900	-1.96117300	0.00000000
Mg10	-1.52277500	-1.53204400	2.28719400	Mg10	-1.52374700	-1.52968200	2.27227800

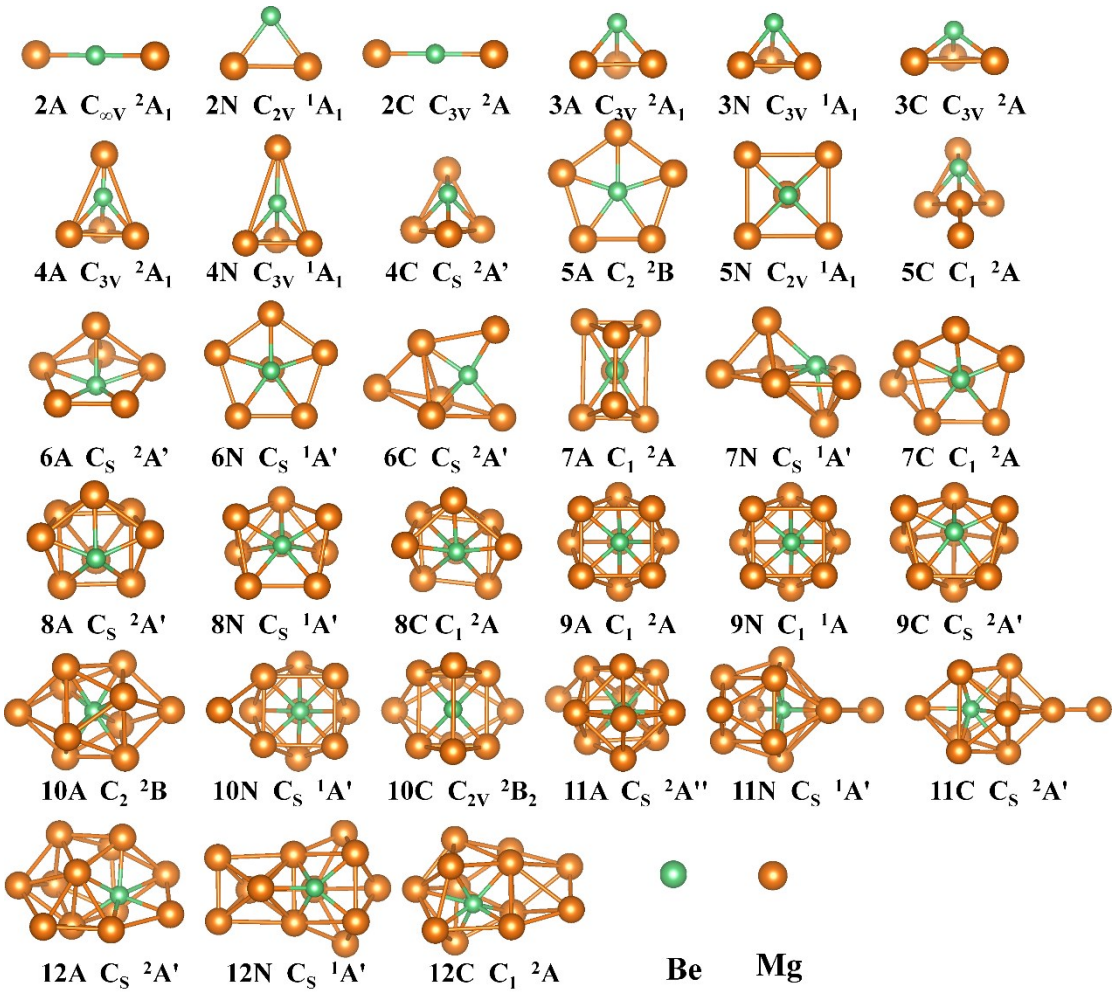

Figure S1. Geometries of the lowest total energy state of $BeMg_n^Q$ (Q = 0, ±1; n = 2 – 12) clusters at PBE0 /6-311G(d, p) level.

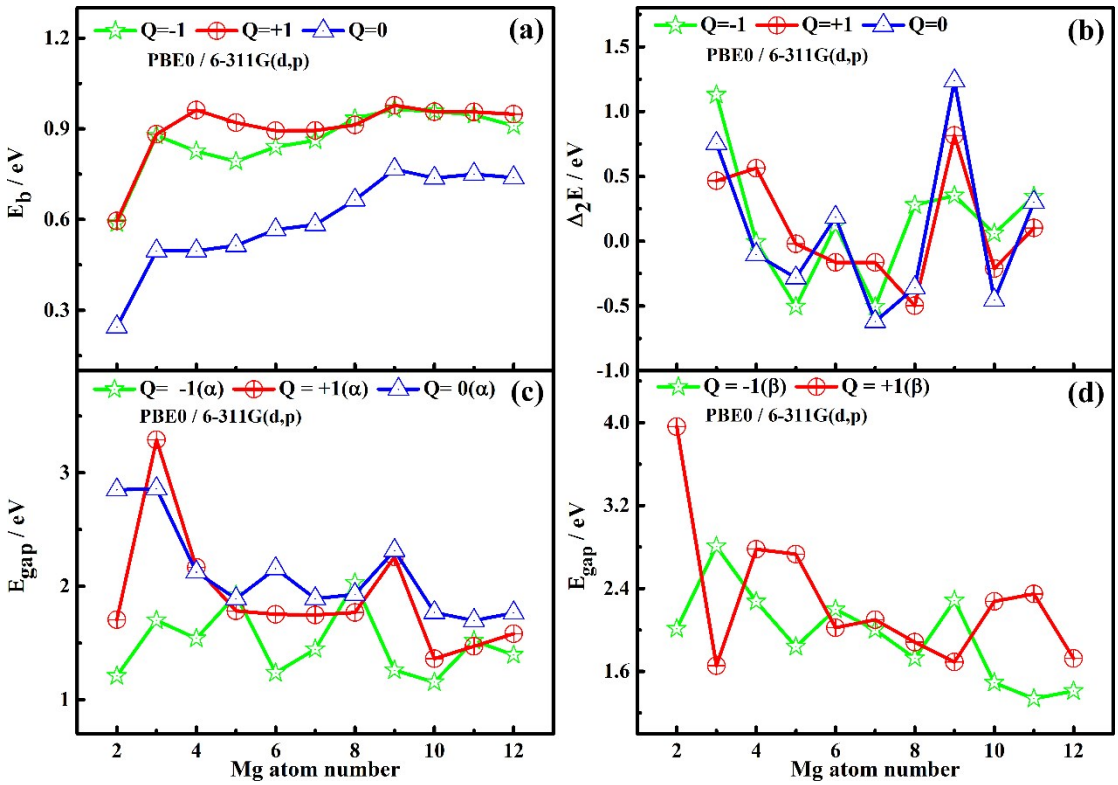

Figure S2. Size dependence of $BeMg_n^Q$ (Q = 0, ±1; n = 2 – 12) clusters' energies at PBE0 / 6-311G (d, p) level (a) Average binding energies E_b, (b) the second order differences Δ_2E, (c) α electrons HOMO-LUMO E_{gap}, (d) β electrons HOMO-LUMO E_{gap}.

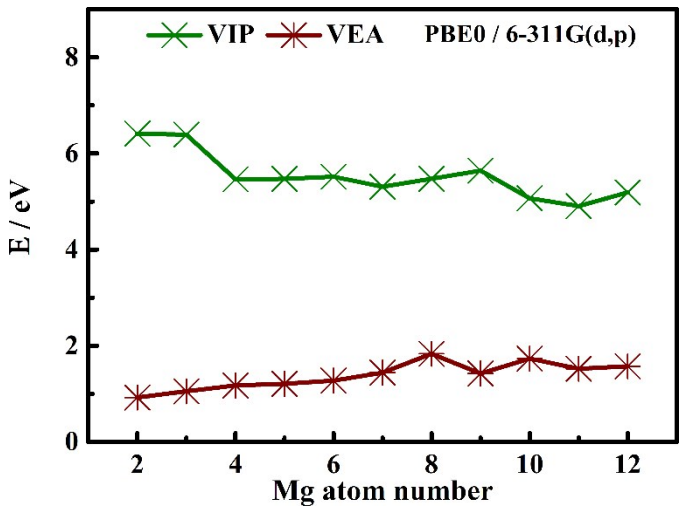

Figure S3. VIP and VEA values of the ground state of $BeMg_n$ (n = 2 -12) clusters at PBE0 / 6-311G(d,p) level.

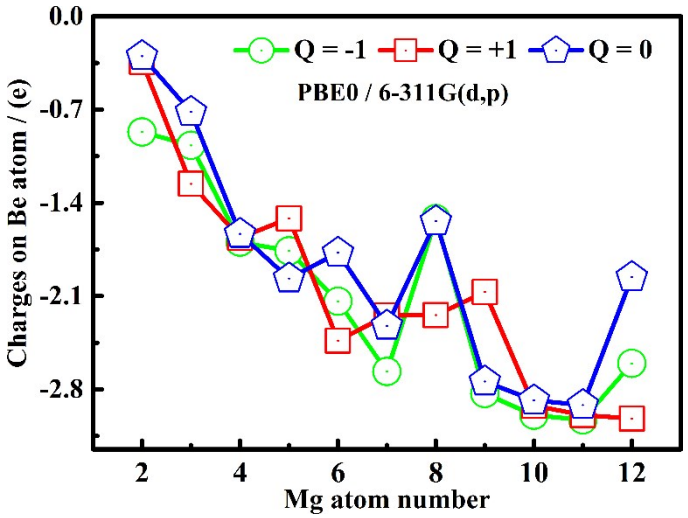

Figure S4. Total charges on Be atoms in the ground state of $BeMg_n^Q$ (Q=0, ±1; n = 2 -12) clusters at PBE0 / 6-311G(d,p) level.

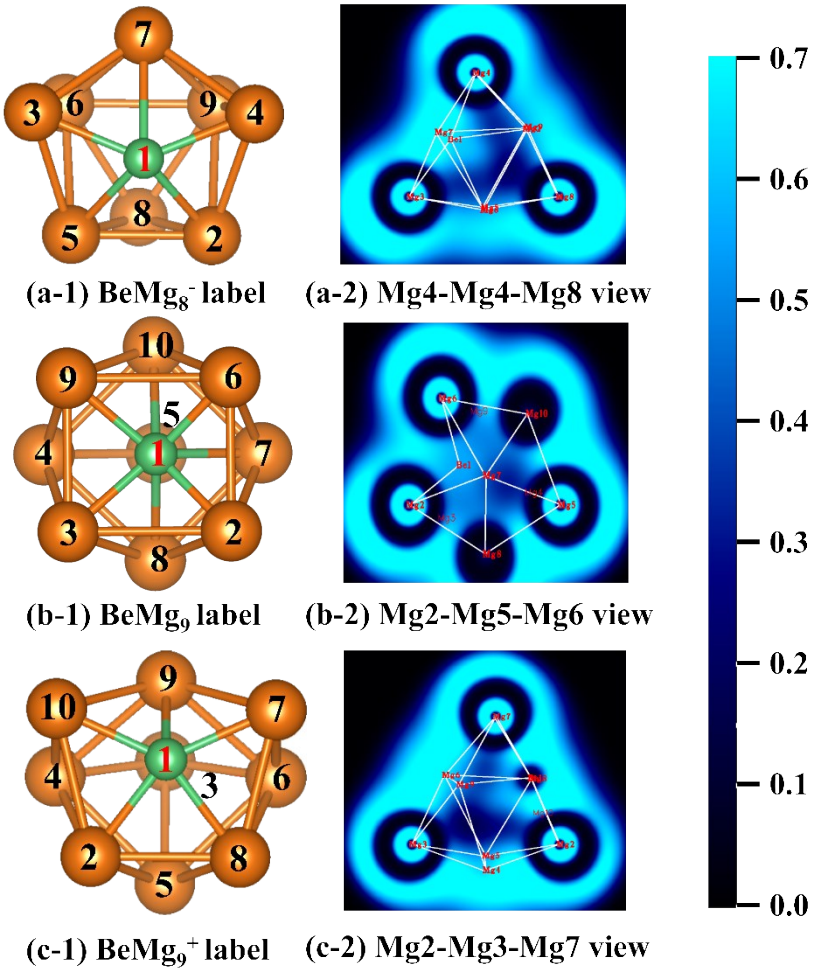

Figure S5. Extra perspective ELF analysis of $BeMg_8^-$, $BeMg_9$, $BeMg_9^+$ clusters at B3PW91/6-311 G(d, p) level.

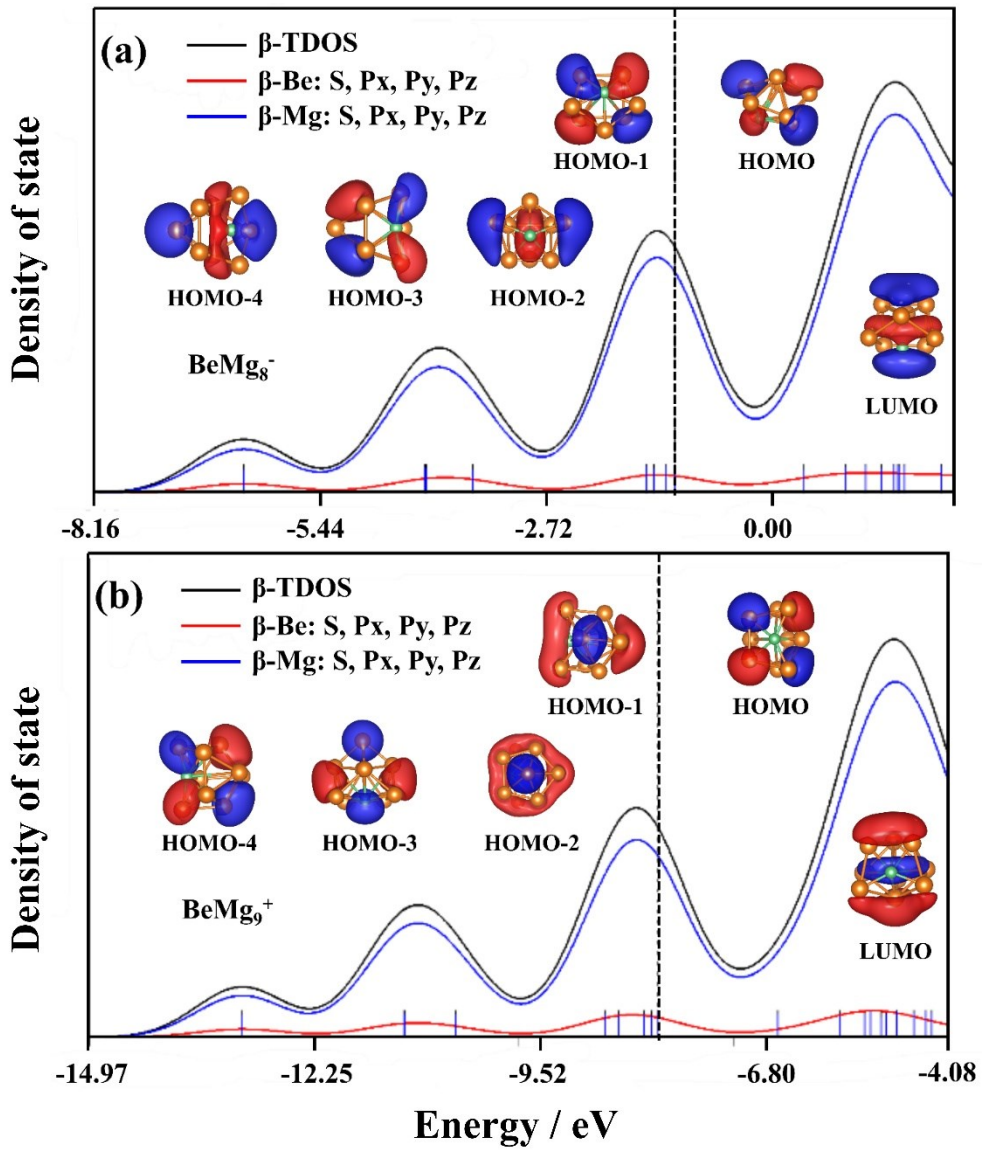

Figure S6. β electrons TDOS and PDOS of $BeMg_8^-$ and $BeMg_9^+$ clusters at B3PW91/6-311 G(d, p) level.