Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Can Alkalide be a Perfect Lewis Base?

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Table S1. CCSD(T)-T_1 diagnostic value on the M06-2X/def2-QZVPP optimized geometries.

System	T_1
$LiBeH_2^-$	0.036
$NaBeH_2^-$	0.045
$KBeH_2^-$	0.058
$LiMgH_2^-$	0.019
$NaMgH_2^-$	0.024
$KMgH_2^-$	0.038
$LiCaH_2^-$	0.016
$NaCaH_2^-$	0.018
$KCaH_2^-$	0.024
$NaBH_3^{-a}$	**0.090**
$NaBH_3^{-b}$	**0.046**

[a] Without broken symmetry. [b] with broken symmetry.

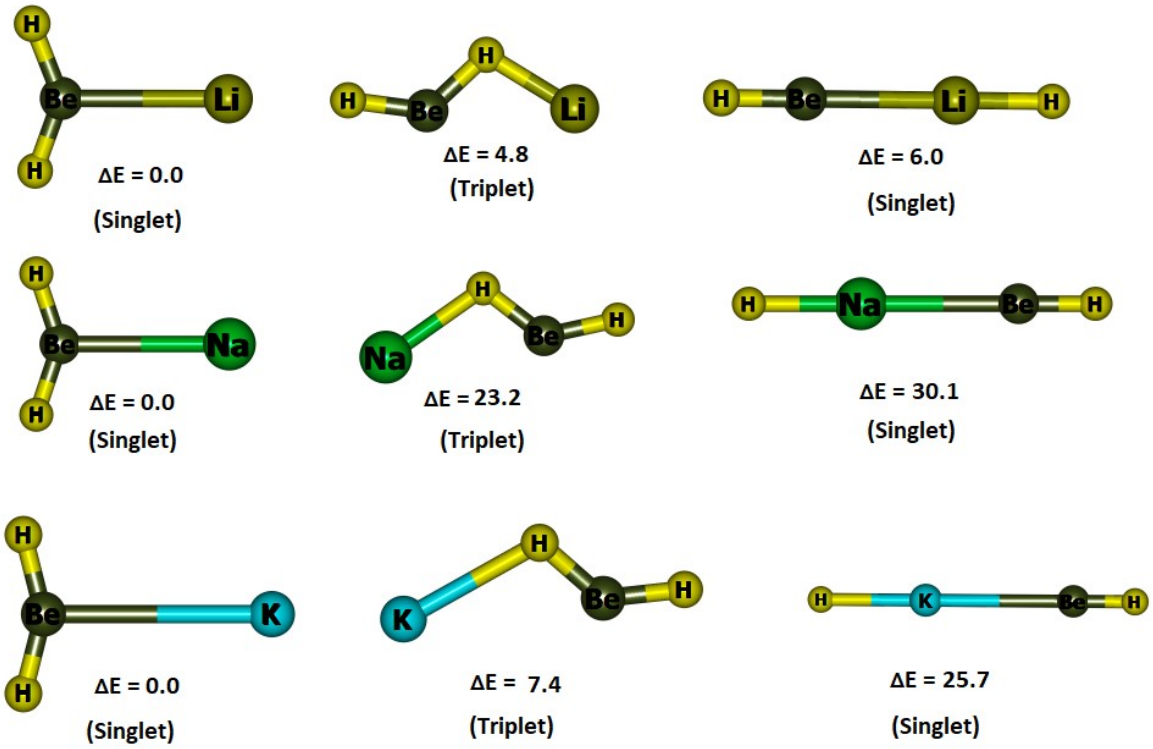

Figure S1. Low energy isomers of $LiBeH_2^-$, $NaBeH_2^-$ and $KBeH_2^-$ clusters along with their relative energies (kcal/mol) calculated at M06-2X/def2-QZVPP + ZPE level.

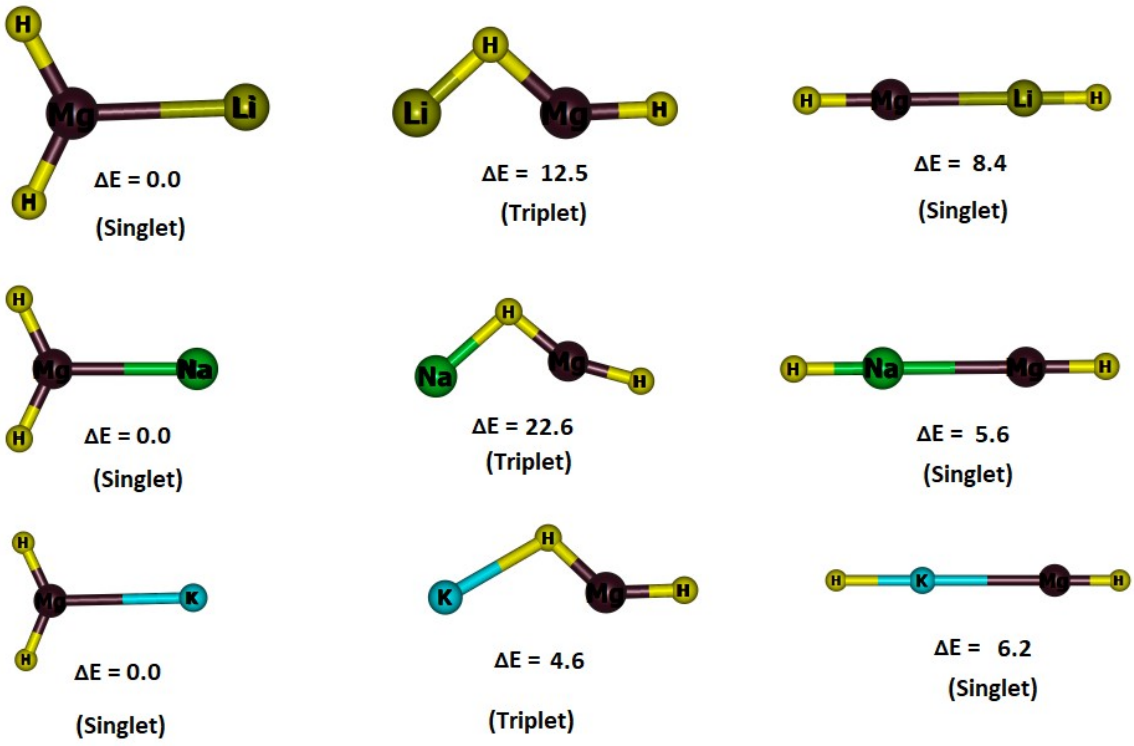

Figure S2. Low energy isomers of $LiMgH_2^-$, $NaMgH_2^-$ and $KMgH_2^-$ clusters along with their relative energies (kcal/mol) calculated at M06-2X/def2-QZVPP + ZPE level.

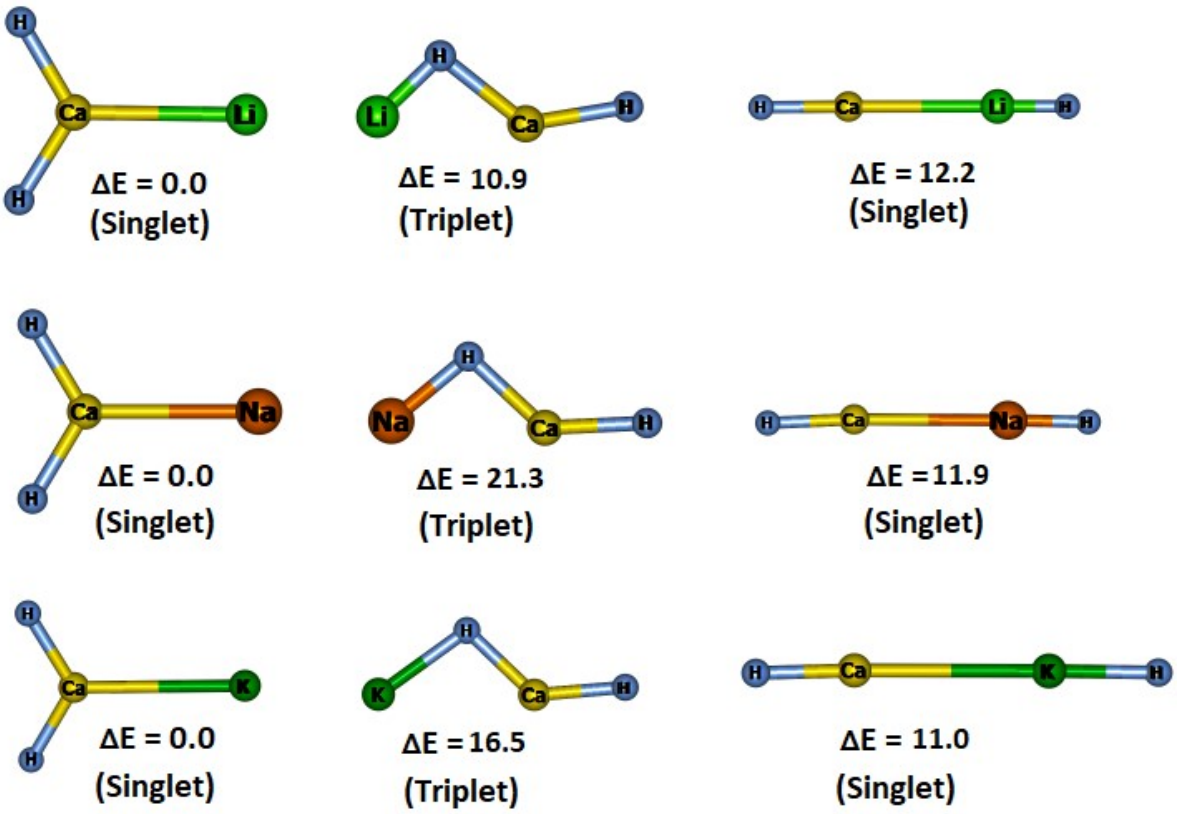

Figure S3. Low energy isomers of $LiCaH_2^-$, $NaCaH_2^-$ and $KCaH_2^-$ clusters along with their relative energies (kcal/mol) calculated at M06-2X/def2-QZVPP + ZPE level.

Cartesian coordinates of the M06-2X/def2-QZVPP optimized geometries.

$LiBeH_2^-$

4	-0.844470000	0.000000000	-0.000065000
1	-1.319882000	-1.271658000	0.000112000
1	-1.319880000	1.271659000	0.000112000
3	2.005881000	0.000000000	0.000012000

$NaBeH_2^-$

4	-1.943521000	0.000000000	-0.000006000
1	-2.370494000	-1.281620000	0.000008000
1	-2.370490000	1.281622000	0.000008000
11	1.137733000	0.000000000	0.000001000

$KBeH_2^-$

4	-2.822112000	0.000000000	-0.000239000
1	-3.150158000	-1.300044000	-0.000246000
1	-3.150154000	1.300045000	-0.000246000
19	0.925724000	0.000000000	0.000076000

$LiMgH_2^-$

12	-0.450612000	0.000000000	0.000000000
1	-1.252330000	-1.567740000	0.000001000
1	-1.252328000	1.567741000	0.000001000
3	2.637333000	0.000000000	0.000000000

$NaMgH_2^-$

12	-1.374243000	0.000000000	-0.000100000
1	-2.132823000	-1.578011000	0.000485000
1	-2.132821000	1.578012000	0.000485000
11	1.886960000	0.000000000	0.000021000

$KMgH_2^-$

12	-2.148453000	0.000000000	0.000001000
1	-2.855585000	-1.592562000	0.000002000
1	-2.855582000	1.592563000	0.000002000
19	1.657505000	0.000000000	-0.000001000

$LiCaH_2^-$

20	-0.328584000	0.000000000	0.000000000
1	-1.409194000	-1.793285000	0.000001000
1	-1.409194000	1.793285000	0.000001000
3	3.130020000	0.000000000	-0.000003000

$NaCaH_2^-$

20	0.000000000	1.123115000	0.000000000
1	-0.000007000	2.196890000	1.790130000
1	-0.000007000	2.196890000	-1.790130000
11	0.000000000	-2.441461000	0.000000000

$KCaH_2^-$

20	0.000000000	1.831688000	0.000000000
1	0.000000000	2.893342000	1.791672000
1	0.000000000	2.893342000	-1.791672000
19	0.000000000	-2.232654000	0.000000000