Supporting Information

Of

Chemical Bonding Misnomer in AeF^- (Ae = Be-Ca) Anions

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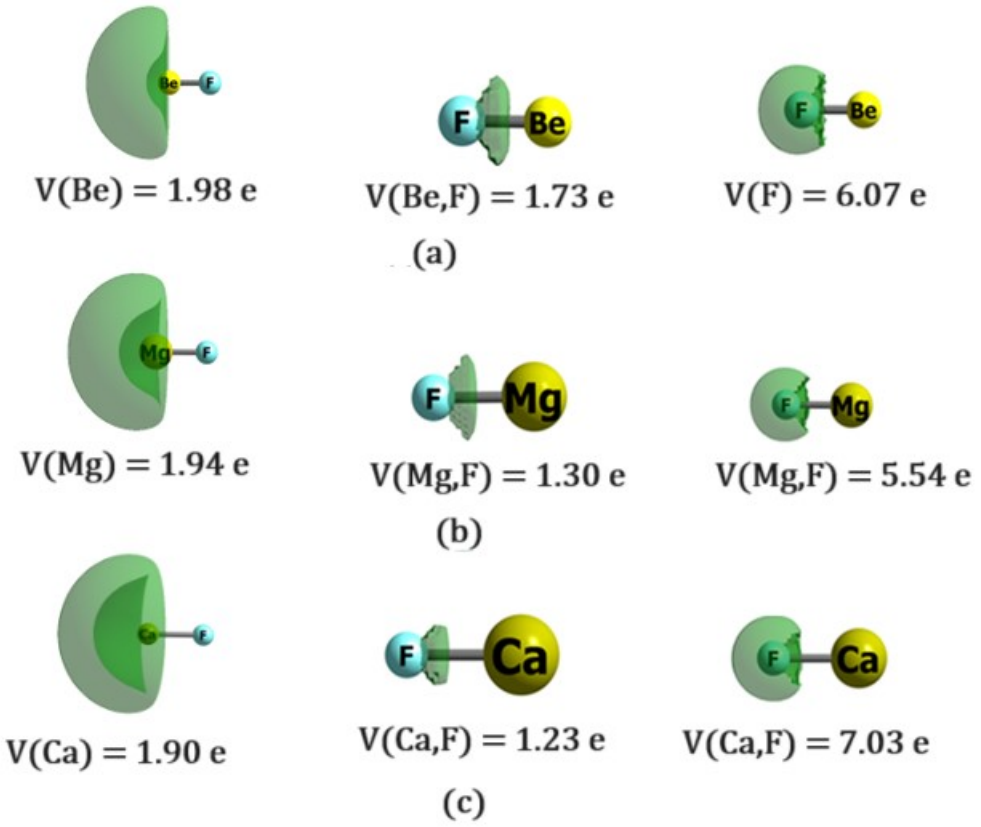

Fig S1. ELF basin iso-surface of (a) BeF^-, (b) MgF^- and (c) CaF^- molecules calculated at HF/def2-QZVPP level. Populations of the basins are in electrons (e). ELF plots were prepared using $\eta = 0.62$ a.u.

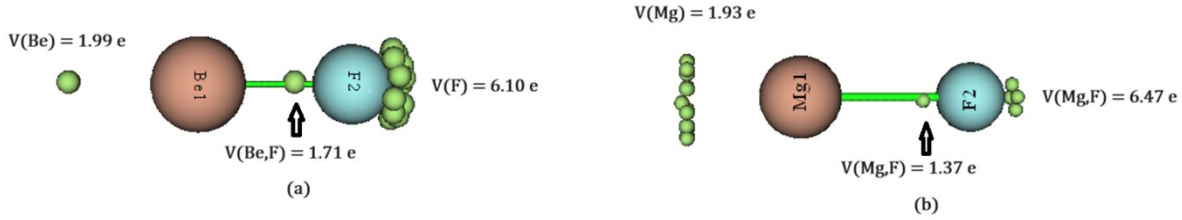

Fig S2. ELF basin populations (in e) and location of attractors for (a) BeF^- and (b) MgF^- molecules calculated at CCSD(T)(Full)/def2-QZVPP level.

Cartesian coordinates of the molecules calculated at CCSD(T)(Full)/def2-QZVPP level along with the total (SCF) energies (a. u).

BeF^-

SCF = -114. 58128

Be	0.000000000	0.000000000	-0.989691000
F	0.000000000	0.000000000	0.439863000

MgF^-

SCF = -299.762834

Mg 0.000000000 0.000000000 0.788573000

F 0.000000000 0.000000000 -1.051431000

CaF^-

SCF = -776.99116

Ca 0.000000000 0.000000000 0.653230000

F 0.000000000 0.000000000 -1.451621000