Supporting Information

Of

Strong Beryllium - Beryllium Bond

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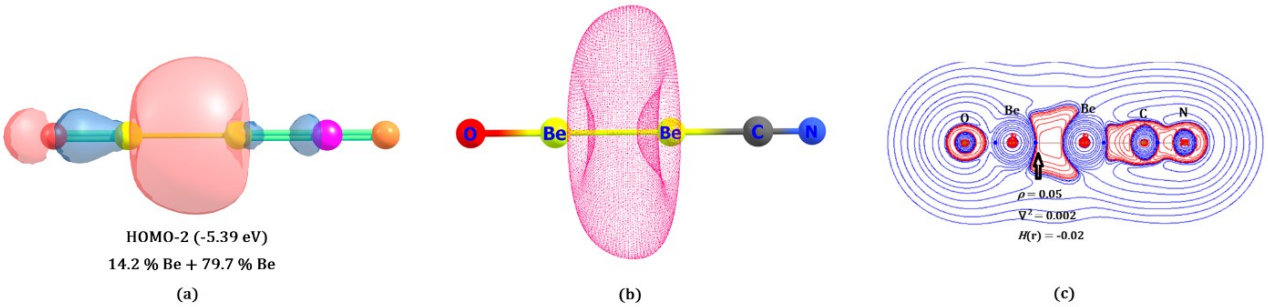

Fig S1. (a) Occupied frontier orbital responsible for Be → Be dative bond along with natural localized molecular (NLMO) composition, (b) ELF V(Be,Be) basin and (c) Laplacian plot of electron density (red = charge concentration; blue = charge depletion). Atoms in molecules parameters are in au. Bond critical point is shown in blue dot.

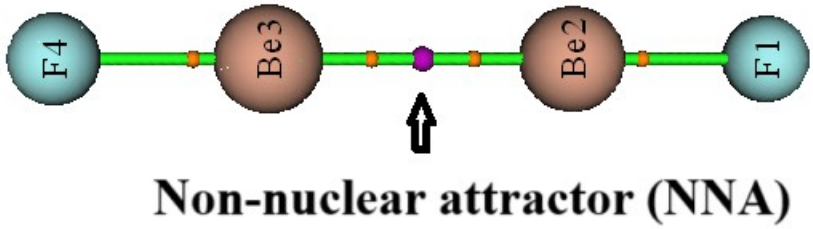

Fig S2. Molecular graph of FBeBeF molecule showing non-nuclear attractor (NNA).

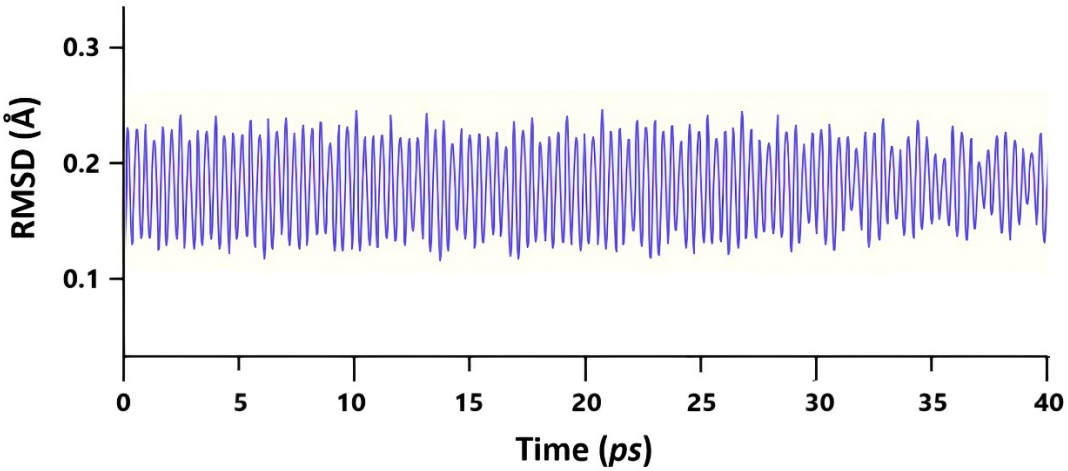

Fig S3. Root-mean-square deviation (Å) versus time (ps) plot obtained through BOMD simulation for $[OBeBeF]^-$ complex.

Cartesian coordinates, lowest vibrational frequency (cm^{-1}) and electronic energies calculated at CCSD(T)/cc-pVTZ level.

[BeO]

ν_1= 1459 cm^{-1}

Sum of electronic and zero-point Energies= -89.744831

Sum of electronic and thermal Energies= -89.742464

Sum of electronic and thermal Enthalpies= -89.741520

Sum of electronic and thermal Free Energies= -89.763961

4	0.000000000	0.000000000	-0.900192000
8	0.000000000	0.000000000	0.450096000

$[BeF]^-$

ν_1= 1063 cm^{-1}

Sum of electronic and zero-point Energies= -114.475798

Sum of electronic and thermal Energies= -114.473409

Sum of electronic and thermal Enthalpies= -114.472464

Sum of electronic and thermal Free Energies= -114.495255

4	0.000000000	0.000000000	-0.988002000
9	0.000000000	0.000000000	0.439112000

[BeF]

ν_1= 1259 cm^{-1}

Sum of electronic and zero-point Energies= -114.445054

Sum of electronic and thermal Energies= -114.442680

Sum of electronic and thermal Enthalpies= -114.441736

Sum of electronic and thermal Free Energies= -114.465094

4	0.000000000	0.000000000	-0.941397000
9	0.000000000	0.000000000	0.418399000

[FBeBeF]

ν_1= 148 cm^{-1}

Sum of electronic and zero-point Energies= -229.009437

Sum of electronic and thermal Energies= -229.004657

Sum of electronic and thermal Enthalpies= -229.003713

Sum of electronic and thermal Free Energies= -229.033877

4	0.000000000	0.000000000	1.023953000
4	0.000000000	0.000000000	-1.023953000
9	0.000000000	0.000000000	-2.397102000
9	0.000000000	0.000000000	2.397102000

$[OBeBeF]^-$

ν_1= 142 cm^{-1}

Sum of electronic and zero-point Energies= -204.387593

Sum of electronic and thermal Energies= -204.382826

Sum of electronic and thermal Enthalpies= -204.381882

Sum of electronic and thermal Free Energies= -204.412573

8	0.000000000	0.000000000	-2.514972000
4	0.000000000	0.000000000	-1.141602000
4	0.000000000	0.000000000	0.930309000
9	0.000000000	0.000000000	2.329438000

[OBeBeCN]$^-$

ν_1 = 97 cm^{-1}

Sum of electronic and zero-point Energies= -197.233352

Sum of electronic and thermal Energies= -197.227411

Sum of electronic and thermal Enthalpies= -197.226467

Sum of electronic and thermal Free Energies= -197.260234

8	0.000000000	0.000000000	3.253963000
4	0.000000000	0.000000000	1.890778000
4	0.000000000	0.000000000	-0.176764000
6	0.000000000	0.000000000	-1.903823000
7	0.000000000	0.000000000	-3.066403000