Effects of the Nanowire Length on Large Second Order Nonlinear Optical Response: A Theoretical Investigation of the Thinnest Doped Beryllium Nanowires with IR and UV Working Wavebands

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Table S1. The static first hyperpolarizability (β_0^e) of $Ca(Be_6)_nMg$ (n=2,3) calculated by different methods and the same basis 6-311+G(d).

β_0^e	$Ca(Be_6)_2Mg$	$Ca(Be_6)_3Mg$
MP2	1.45×10^4	4.61×10^4
B3LYP	1.90×10^4	2.16×10^4
CAM-B3LYP	1.93×10^4	2.60×10^4
BHandHLYP	**1.82×10^4**	**2.67×10^4**
M06-2X	2.44×10^4	9.33×10^3

Table S2. The static first hyperpolarizability (β_0^e) of $Ca(Be_6)nMg$ (n=2,3) calculated by the same BHandHLYP method and different basis sets.

β_0^e	$Ca(Be_6)_2Mg$	$Ca(Be_6)_3Mg$
6-31+G	1.34×10^4	2.05×10^4
6-31+G(d)	1.56×10^4	2.33×10^4
6-31+G(d,p)	1.56×10^4	2.33×10^4
6-31++G(d,p)	1.56×10^4	2.33×10^4
6-311+G(d)	**1.82×10^4**	**2.67×10^4**
6-311+G(d,p)	1.82×10^4	2.67×10^4
6-311++G(d,p)	1.82×10^4	2.67×10^4
6-311++G(2d,2p)	1.82×10^4	2.67×10^4
6-311++G(2df,2pd)	1.85×10^4	2.73×10^4

Table S3. The valences (V), Static Electronic First Hyperpolarizability β_0^e (au), Electronic spatial extent <R^2> (au) and Polarizability α^e(au).

Systems	V	β_0^e	<R^2>	α^e
$(Be_6)_4$	0	0.0019×10^4	5.78×10^3	8.15×10^2
$Li(Be_6)_4$	-1	2.45×10^4	6.40×10^3	8.59×10^2
$Mg(Be_6)_4$	-2	1.73×10^4	8.22×10^3	9.84×10^2
$Li(Be_6)_4Mg$	-3	1.71×10^4	9.06×10^3	9.91×10^2
$Na(Be_6)_4Mg$	-3	2.64×10^4	11.1×10^3	10.3×10^2
$Ca(Be_6)_4Mg$	-4	3.98×10^4	13.4×10^3	15.3×10^2

The electronic spatial extent <R^2> is a physical property which characterizes the electron density volume around the molecule.[66]

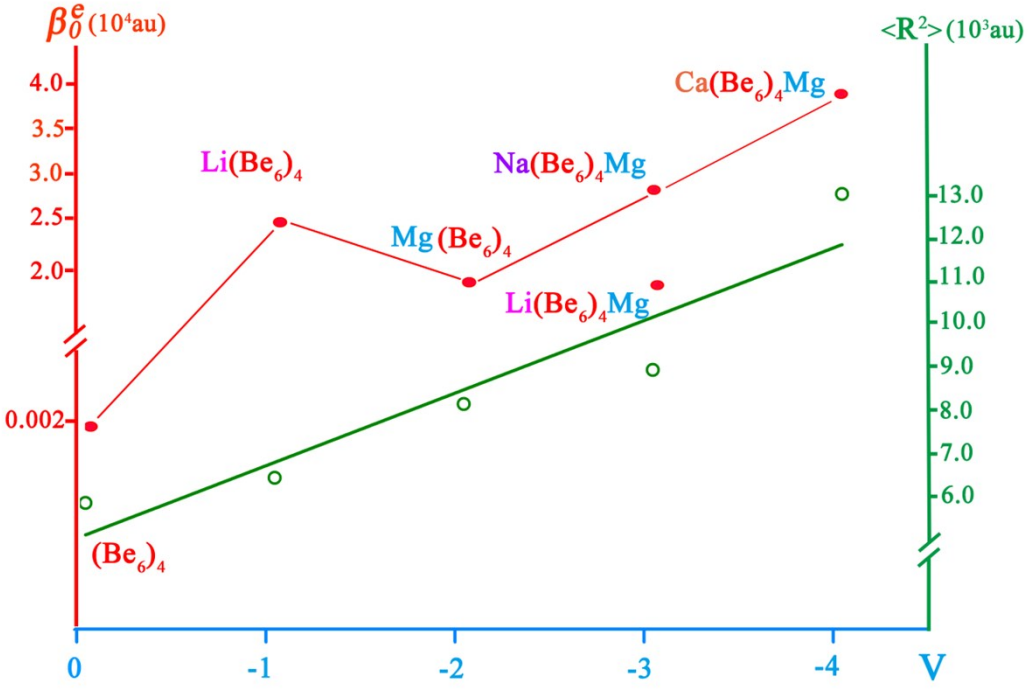

Figure S1. The V value dependences on β_0^e and <R^2>.

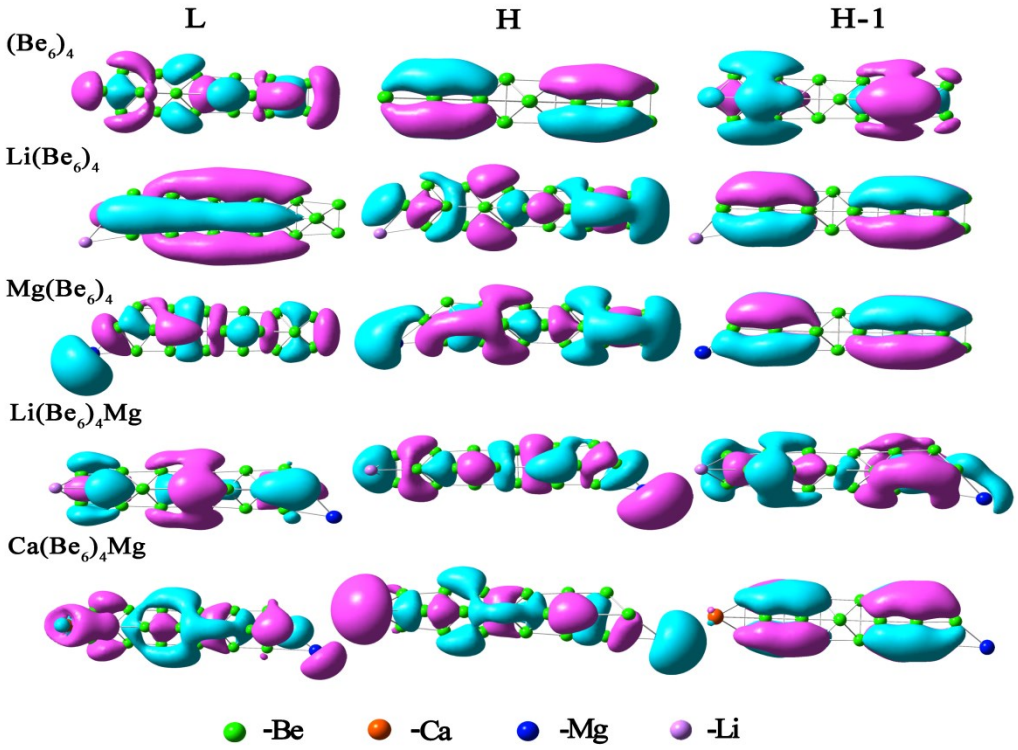

Figure S2. Frontier orbitals and occupied orbitalsof for $(Be_6)_4$ chains and corresponding doped $Li(Be_6)_4$, $Mg(Be_6)_4$, $Li(Be_6)_4Mg$ and $Ca(Be_6)_4Mg$.