Designing Molecular Electrides from Defective Unit Cells of Cubic Alkaline Earth Oxides.

Supporting Information

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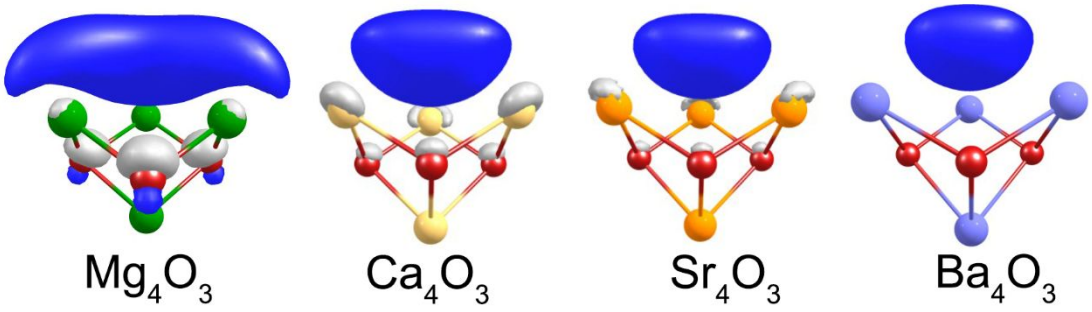

Figure S1. HOMOs of studied structures. Contour value is 0.043.

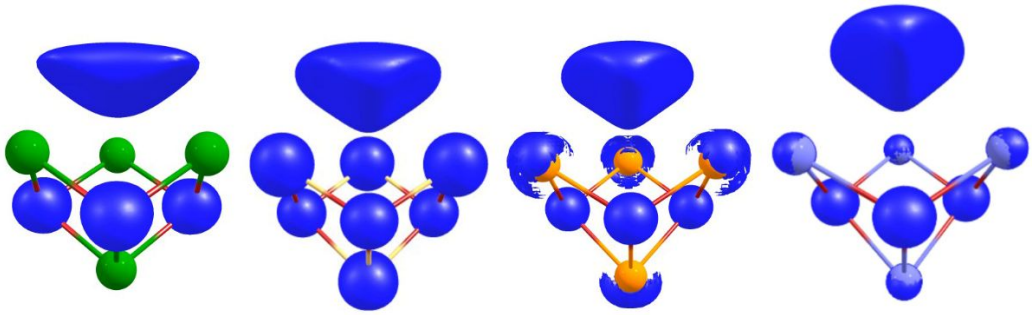

Figure S2. LOL isosurfaces of studied structures. Isovalue = 0.5. (PBE0-DKH/aug-cc-pVTZ-DK).

Table S1. GM of Be_4O_3

4	2.141356000	0.844043000	0.979691000

4	-0.496011000	2.611644000	0.860034000
4	1.700912000	3.102590000	0.459846000
4	-0.110812000	0.636626000	1.314900000
8	1.105869000	-0.099888000	1.350026000
8	0.369641000	3.675017000	0.480716000
8	2.726936000	2.099801000	0.586576000

Table S2. GM Mg_4O_3

12	-1.450362000	0.837367000	-0.660272000
12	1.450362000	0.837367000	-0.660272000
12	0.000000000	-1.674734000	-0.660272000
12	0.000000000	0.000000000	1.372196000
8	0.000000000	1.642065000	0.304310000
8	1.422070000	-0.821032000	0.304310000
8	-1.422070000	-0.821032000	0.304310000

Table S3. GM Ca_4O_3

20	1.390745000	-1.389034000	-0.713268000
20	0.507605000	1.898855000	-0.713243000
20	-1.898532000	-0.509797000	-0.713090000
20	0.000012000	-0.000111000	1.711767000
8	-1.198773000	1.197235000	0.356601000
8	-0.437175000	-1.636871000	0.356290000
8	1.636370000	0.439851000	0.356695000

Table S4. GM Sr_4O_3

38	-1.842197000	1.063593000	-0.721511000
38	1.842197000	1.063593000	-0.721511000
38	0.000000000	-2.127186000	-0.721511000
38	0.000000000	0.000000000	1.908382000
8	0.000000000	1.747558000	0.405573000
8	1.513430000	-0.873779000	0.405573000
8	-1.513430000	-0.873779000	0.405573000

Table S5. GM Ba_4O_3

56	-0.000973000	-0.002222000	2.081775000
56	-2.280799000	-0.294909000	-0.753247000
56	0.884701000	2.123714000	-0.750538000
56	1.397057000	-1.826465000	-0.753246000
8	1.757443000	0.227964000	0.410061000
8	-1.075896000	1.407499000	0.409809000
8	-0.681448000	-1.636288000	0.406917000

Table S6. At PBE0-DKH/aug-cc-pVTZ-DK level of theory.

System	<α>, a.u.	β_{tot}, a.u.	Excitation energy, eV
Be_4O_3	66.79	524.61	5.25
Mg_4O_3	243.86	5689.96	2.06
Ca4O3	508.11	37703.84	1.42
Sr4O3	634.175	46218.29	1.31
Ba4O3	837.99	65747.73	1.18

Table S7. Dissociation energy of Ca_4O_3. (PBE0/def2-TZVP + ZPE).

Fragments	Energy, kcal/mol
Ca_2O_2+Ca_2O	378088.9

3xCaO+Ca	298.5
Ca_3O_3+Ca	81.9
Ca_2O+2xCaO	378206.7
Ca_3O_2+CaO	123.8
4Ca+3O	789.3