

Supporting Information

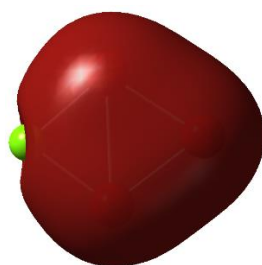
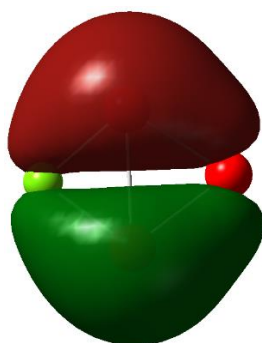
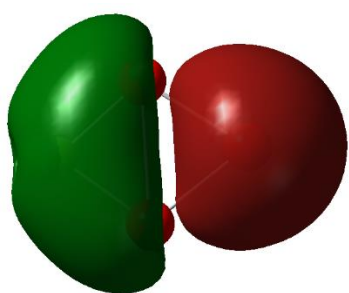
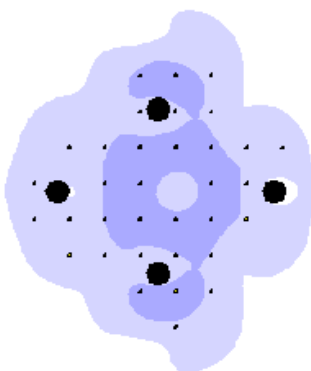
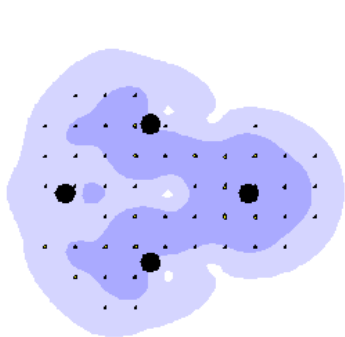
Structures, Thermochemical Properties and Bonding of Mixed Earth-Alkali Silicon Trimers $\text{Si}_3\text{M}^{+/0/-}$ with M = Be, Mg, Ca

Tran Dieu Hang, Huynh Minh Hung, Huyen Thi Nguyen, Minh Tho Nguyen

Department of Chemistry, University of Leuven, B-3001 Leuven, Belgium

Structure	Geometry (Cartesian Coordinates)			
Si_3Be - singlet	14	0.000000000	1.312463000	-0.426772000
	14	0.000000000	0.000000000	1.444855000
	14	0.000000000	-1.312463000	-0.426772000
	4	0.000000000	0.000000000	-2.069590000
Si_3Be - triplet	14	-0.019908000	-0.312501000	1.857735000
	14	-0.019908000	-0.312501000	-1.857735000
	14	-0.019908000	1.009221000	0.000000000
	4	0.209034000	-1.344769000	0.000000000
Si_3Mg - singlet	14	0.000000000	1.350069000	0.027898000
	14	0.000000000	-1.350069000	0.027898000
	14	0.000000000	0.000000000	1.823871000
	12	0.000000000	0.000000000	-2.192946000
Si_3Mg - triplet	14	0.000000000	1.818771000	0.080354000
	14	0.000000000	-1.818771000	0.080354000
	14	0.000000000	0.000000000	1.376601000
	12	0.000000000	0.000000000	-1.793527000
Si_3Ca - singlet	14	0.000000000	1.235625000	-0.368146000
	14	0.000000000	0.000000000	-2.283712000
	20	0.000000000	0.000000000	2.114003000
	14	0.000000000	-1.235625000	-0.368146000
Si_3Ca - triplet	14	0.431436000	-0.743310000	1.275099000
	14	0.431436000	-0.743310000	-1.275099000
	14	-1.479210000	-0.622642000	0.000000000
	20	0.431436000	1.476483000	0.000000000

Si₃Be

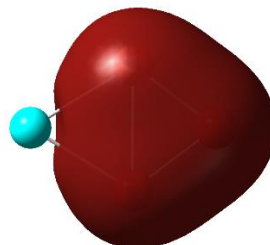
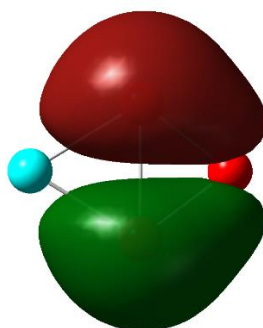
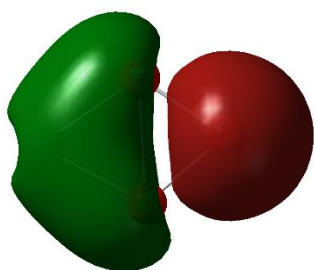
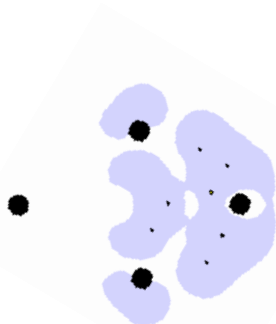
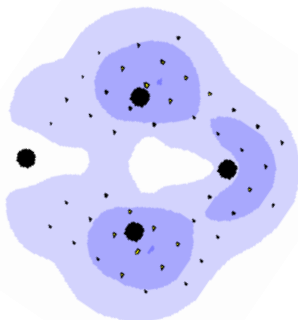
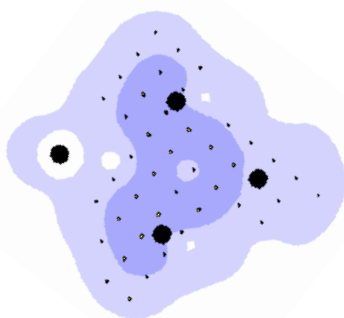


HOMO-4a1

HOMO-5b3

HOMO-6b1

Si₃Mg

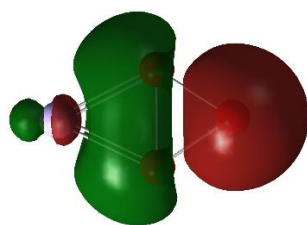
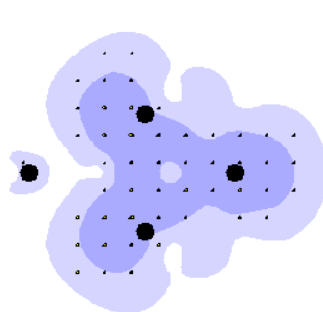


HOMO-4a1

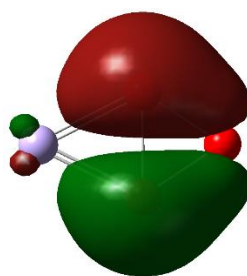
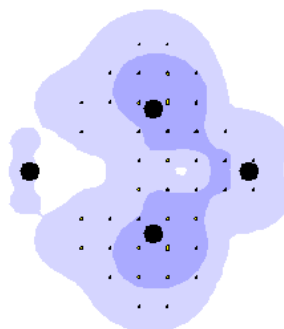
HOMO-5b2

HOMO-6a1

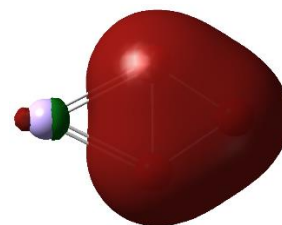
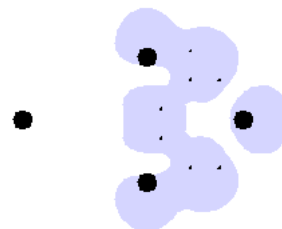
Si₃Ca



HOMO-4a1



HOMO-5b2



HOMO-6a1