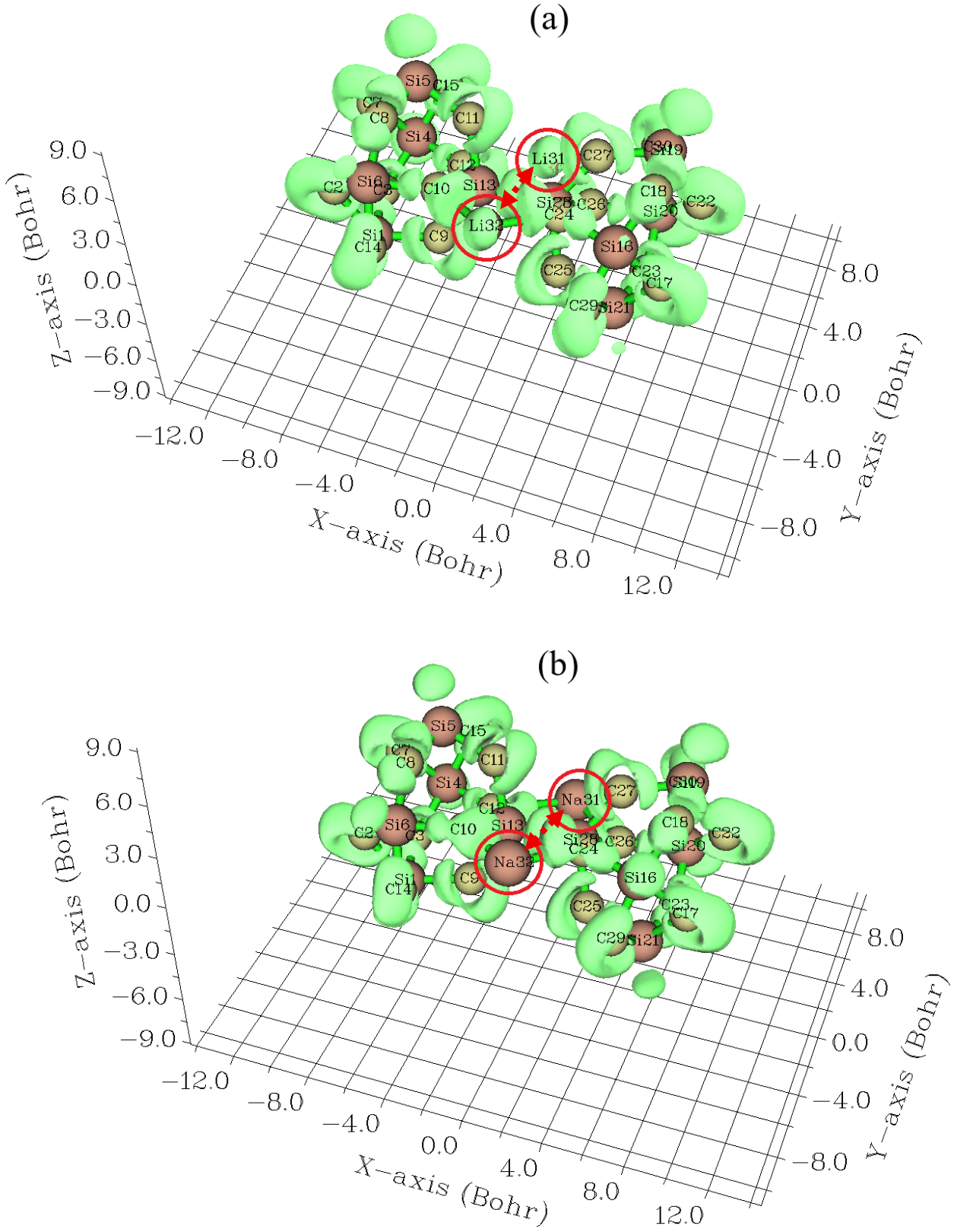
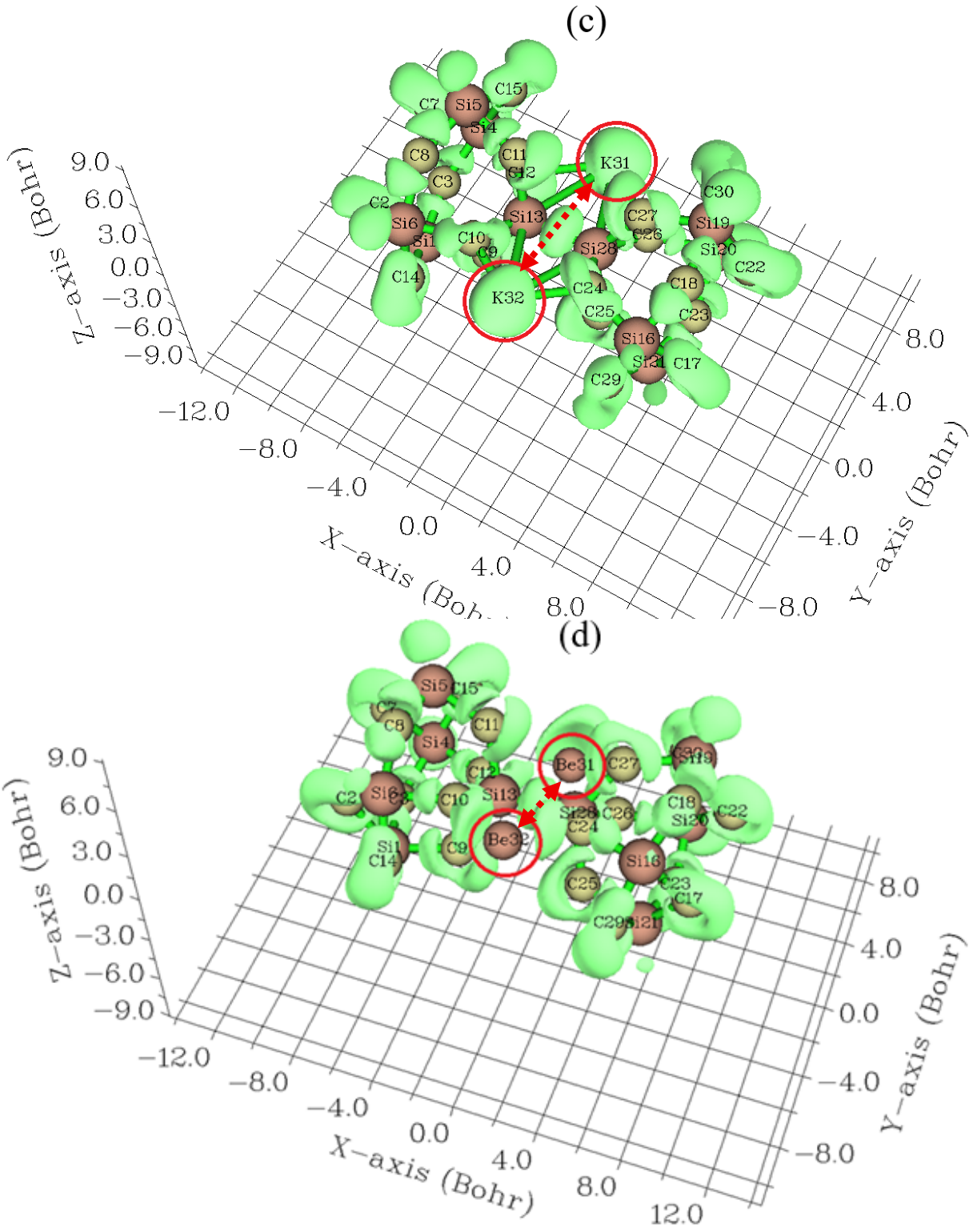
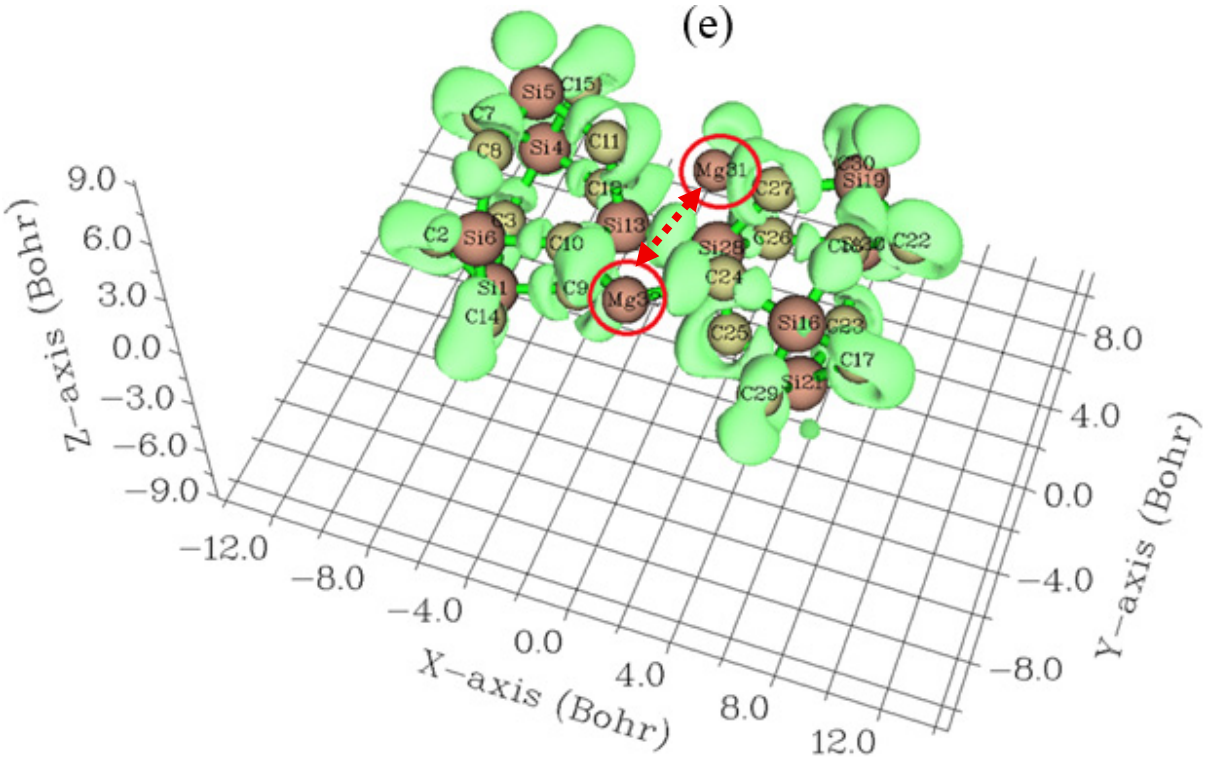
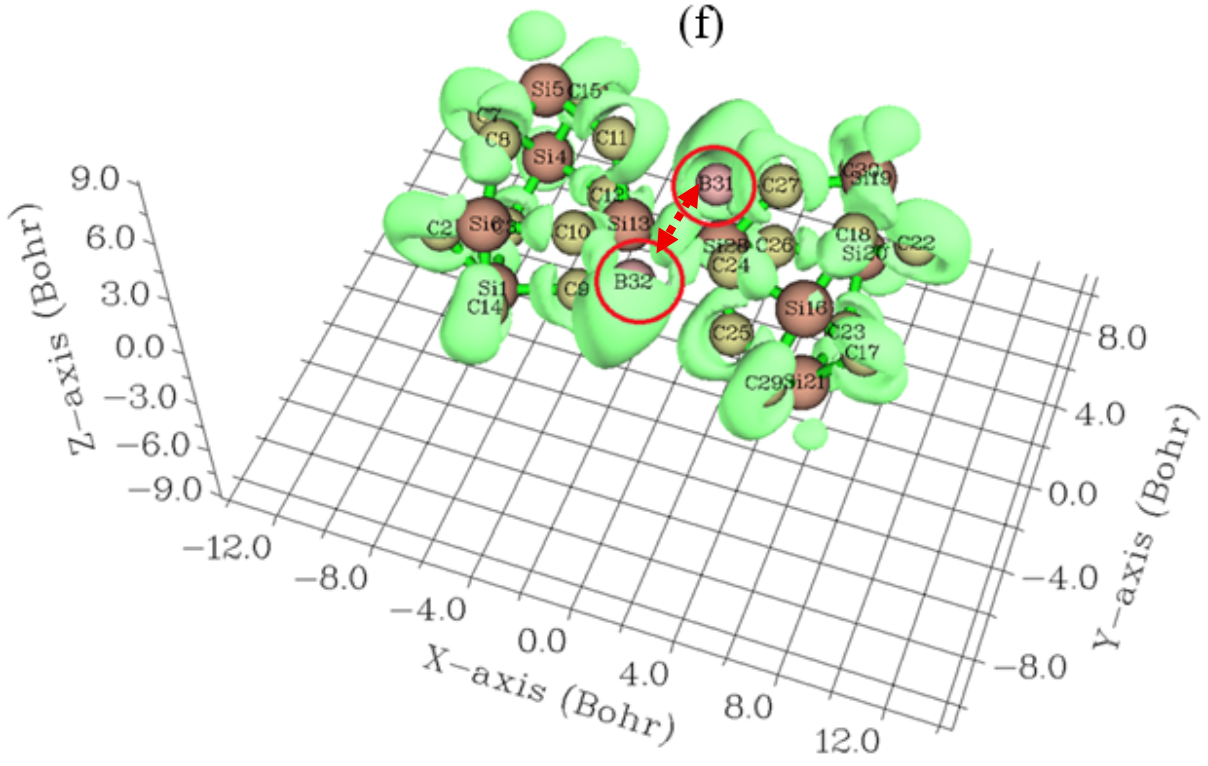

(a)
Z−axis (Bohr)
9.0
6.0
3.0
0.0
−3.0
−6.0
−9.0
X−axis (Bohr)
−12.0
−8.0
−4.0
0.0
4.0
8.0
12.0
Y−axis (Bohr)
8.0
4.0
0.0
−4.0
−8.0
Si5
C15
C7
C8
C11
Si4
C12
Li31
C27
Si19
C2
Si6
C3
C10
Si13
Si28
C26
C18
C22
C24
Si20
Si1
C14
C9
Li32
Si16
C25
C23
C17
C29
Si21
(b)
Z−axis (Bohr)
9.0
6.0
3.0
0.0
−3.0
−6.0
−9.0
X−axis (Bohr)
−12.0
−8.0
−4.0
0.0
4.0
8.0
12.0
Y−axis (Bohr)
8.0
4.0
0.0
−4.0
−8.0
Si5
C15
C7
C8
C11
Si4
C12
Na31
C27
Si19
C2
Si6
C3
C10
Si13
Si28
C26
C18
C22
C24
Si20
Si1
C14
C9
Na32
Si16
C25
C23
C17
C29
Si21


(c)
C15
C7
Si5
Si14
C8
C11
C12
K31
C3
C30
C2
Si6
Si13
C27
Si19
Si1
C10
C9
Si28
C26
Si20
C22
C14
K32
C24
C18
C25
C23
Si16
Si21
C17
C29
9.0
6.0
3.0
0.0
−3.0
−6.0
−9.0
Z−axis (Bohr)
−12.0
−8.0
−4.0
0.0
4.0
8.0
X−axis (Bohr)
8.0
4.0
0.0
−4.0
−8.0
Y−axis (Bohr)
(d)
Si5
C15
C7
C8
C11
Si14
C12
Be31
C27
C30
Si19
C2
Si6
C10
Si13
C18
C22
Si28
C26
Si20
C24
Si1
C14
C9
Be32
Si16
C25
C23
C17
C29
Si21
9.0
6.0
3.0
0.0
−3.0
−6.0
−9.0
Z−axis (Bohr)
−12.0
−8.0
−4.0
0.0
4.0
8.0
12.0
X−axis (Bohr)
8.0
4.0
0.0
−4.0
−8.0
Y−axis (Bohr)


(e)
Z–axis (Bohr)
9.0
6.0
3.0
0.0
−3.0
−6.0
−9.0
−12.0
−8.0
−4.0
0.0
4.0
8.0
12.0
X–axis (Bohr)
8.0
4.0
0.0
−4.0
−8.0
Y–axis (Bohr)
Si5
C15
C7
C8
Si4
C11
Mg31
C27
Si19
C2
Si6
C10
Si13
Si28
C26
C22
Si1
C9
C24
C14
Si16
C23
C17
C29
Si21


(f)
Z–axis (Bohr)
9.0
6.0
3.0
0.0
−3.0
−6.0
−9.0
−12.0
−8.0
−4.0
0.0
4.0
8.0
12.0
X–axis (Bohr)
8.0
4.0
0.0
−4.0
−8.0
Y–axis (Bohr)
Si5
C15
C7
C8
Si4
C11
B31
C27
Si19
C2
Si6
C10
Si13
C26
C18
Si20
C22
Si1
C9
B32
C24
C14
Si16
C25
C23
C17
C29
Si21

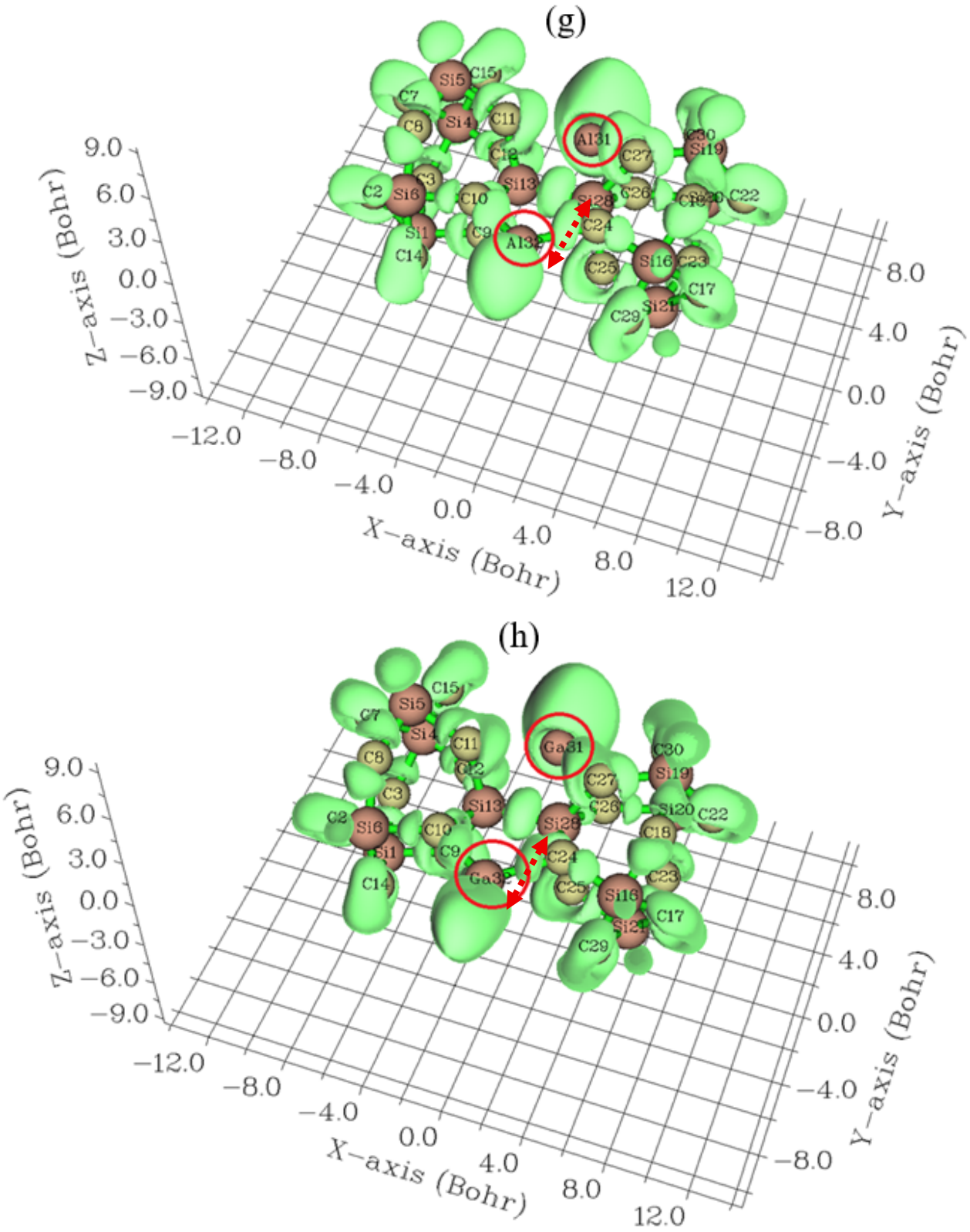
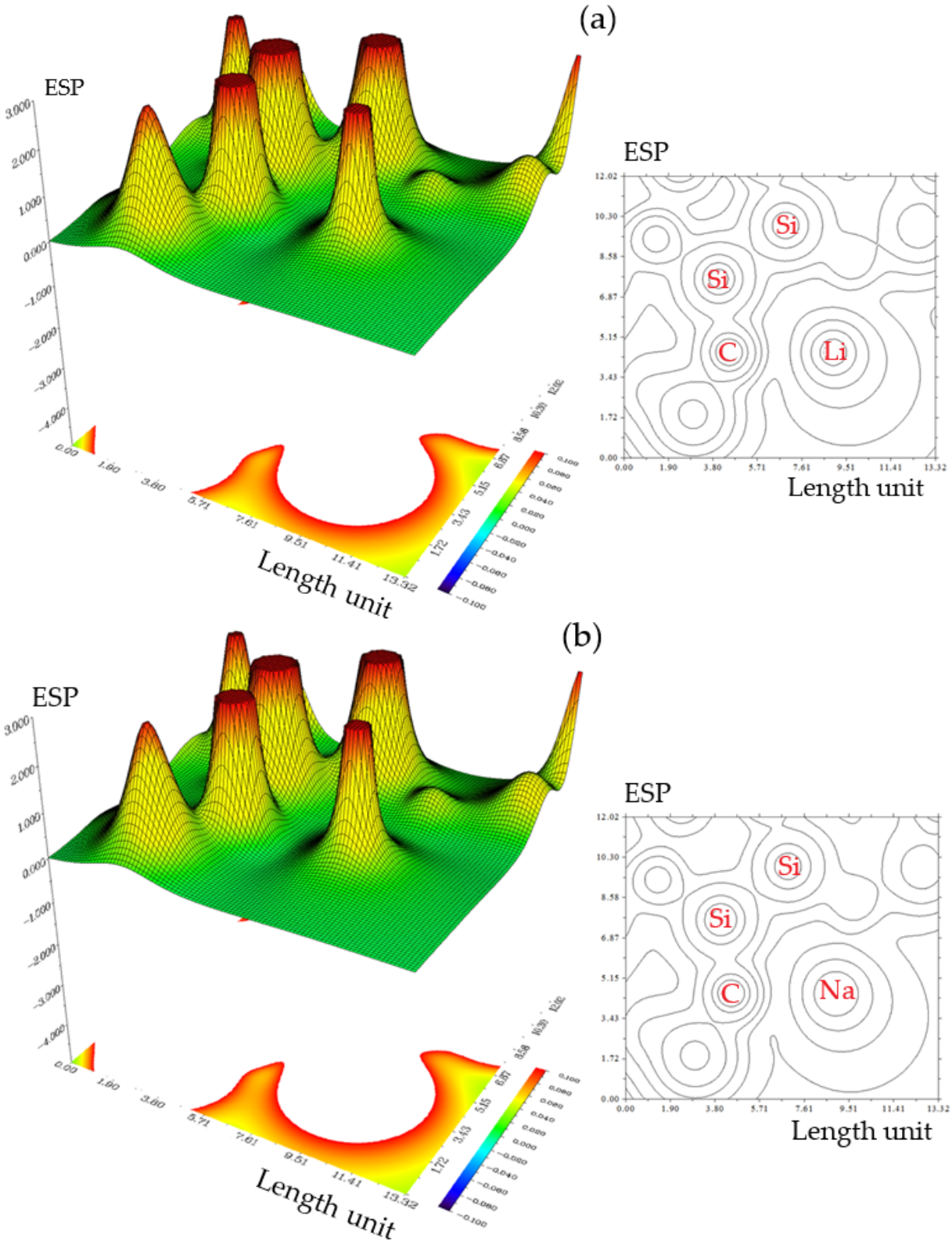
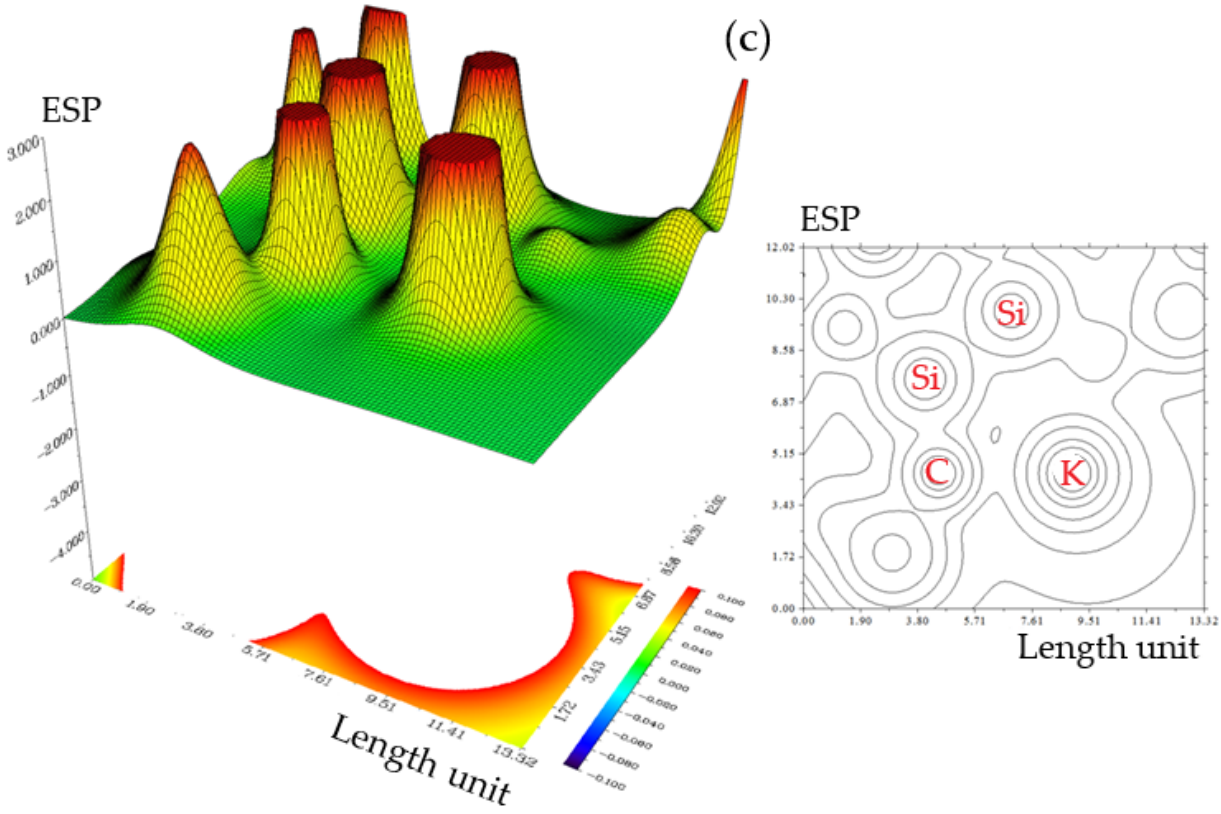
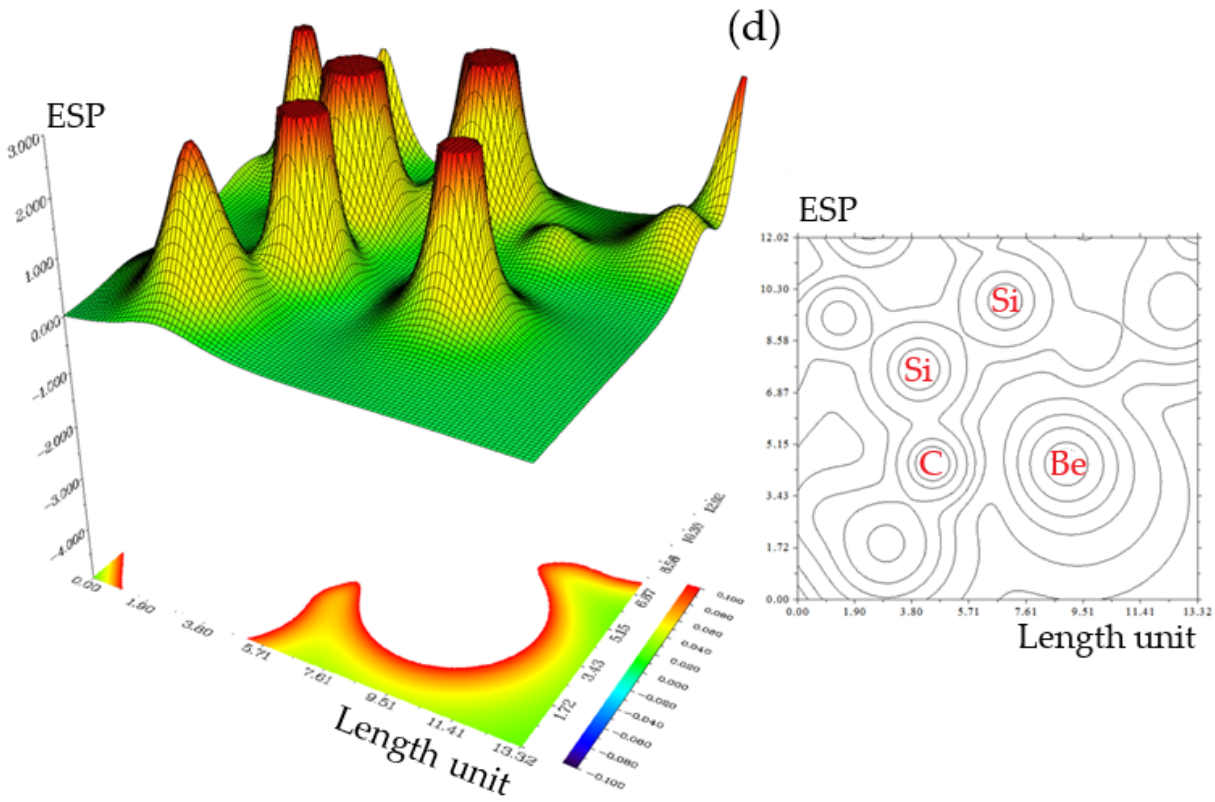
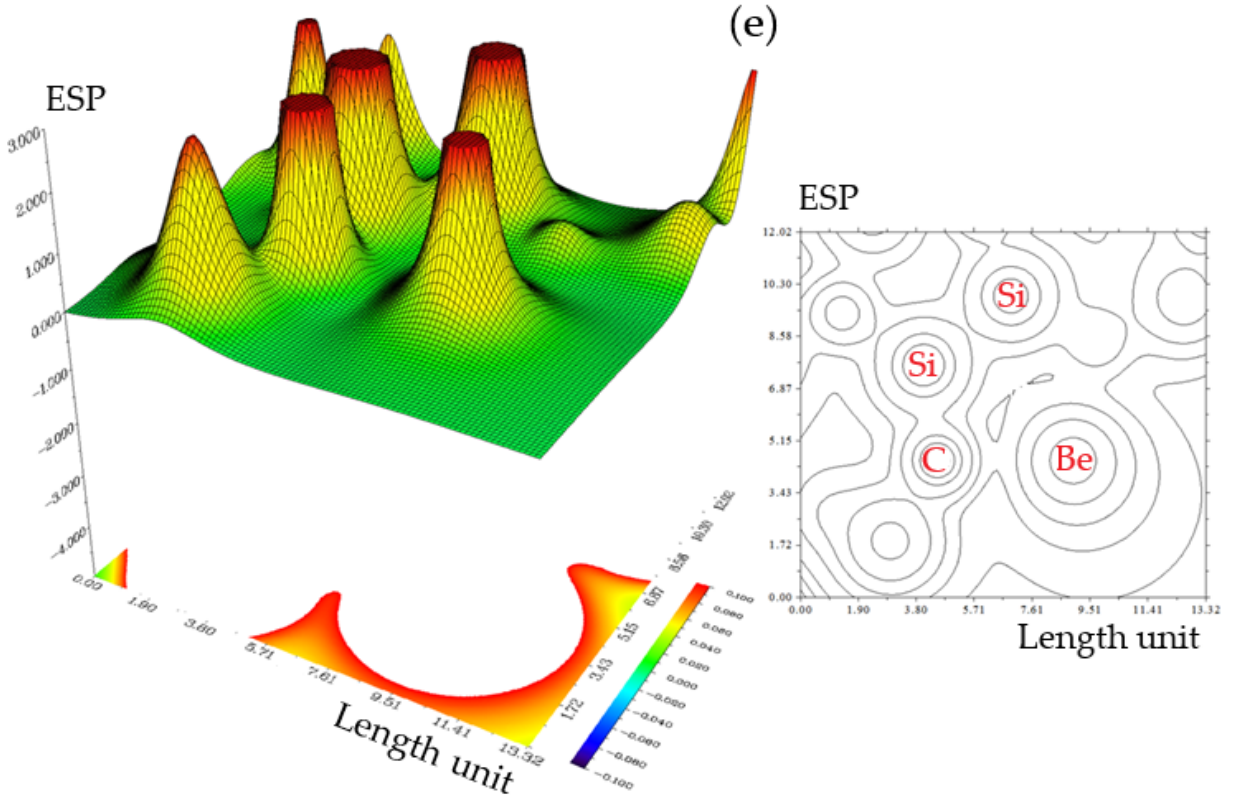


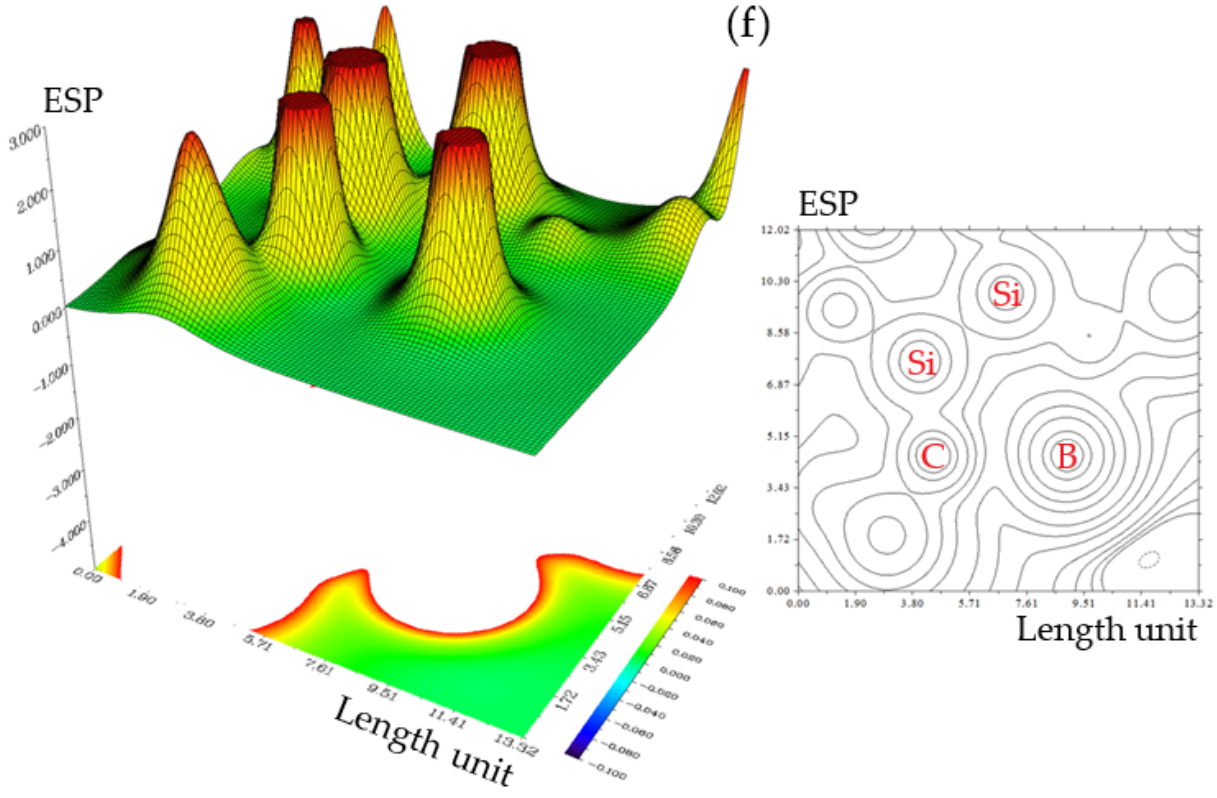
Figure S1. CDD graphs for (a) SiLiC, (b) SiNaC, (c) SiKC, (d) SiBeC, (e) SiMgC, (f) SiBC, (g) SiAlC, (h) SiGaC nanoclusters.

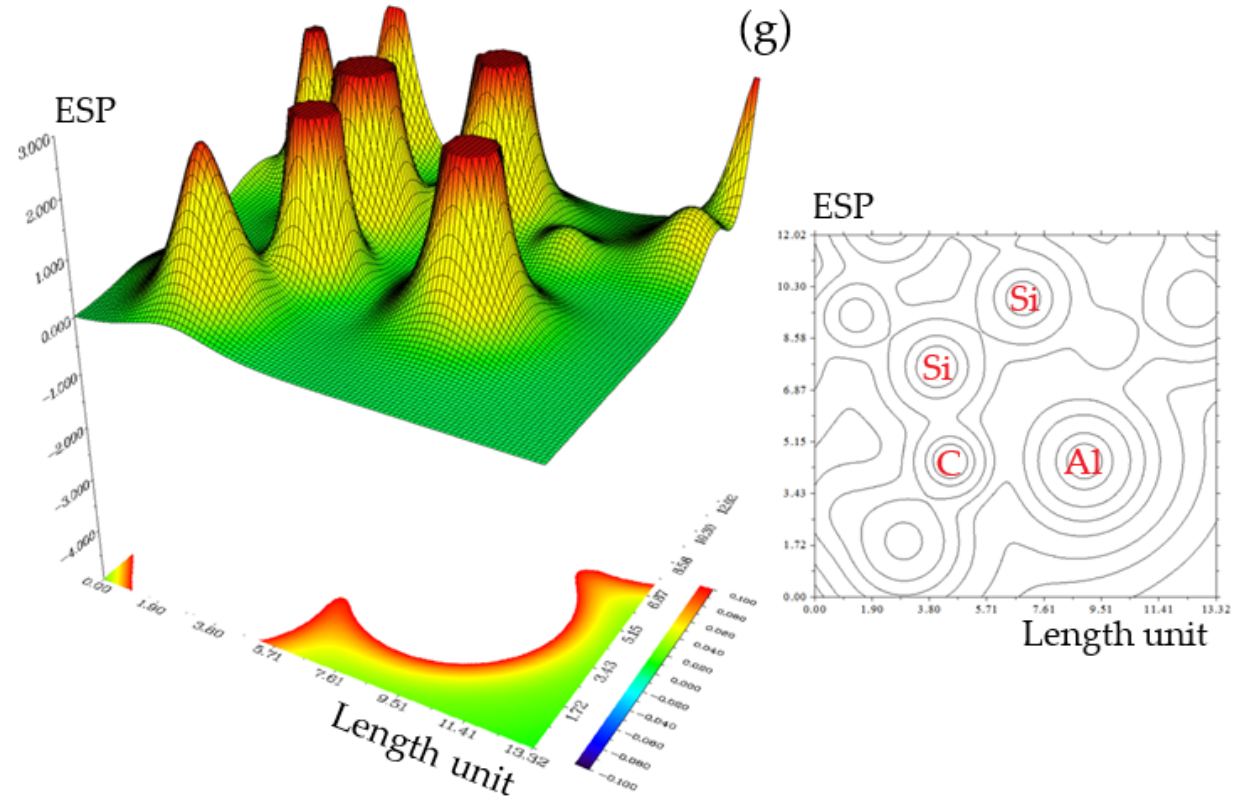

(a)
ESP
3.000
2.000
1.000
0.000
-1.000
-2.000
-3.000
-4.000
0.00
1.60
3.60
5.71
7.61
9.51
11.41
13.32
Length unit
ESP
Si
Si
C
Li
Length unit
(b)
ESP
Si
Si
C
Na
Length unit


(c)
ESP
Length unit
ESP
Si
Si
C
K
Length unit


(d)
ESP
Length unit
ESP
Si
Si
C
Be
Length unit


(e)
ESP
Length unit
ESP
Si
Si
C
Be
Length unit


(f)
ESP
Length unit
ESP
Si
Si
C
B
Length unit


(g)
ESP
Length unit
ESP
Si
Si
C
Al
Length unit

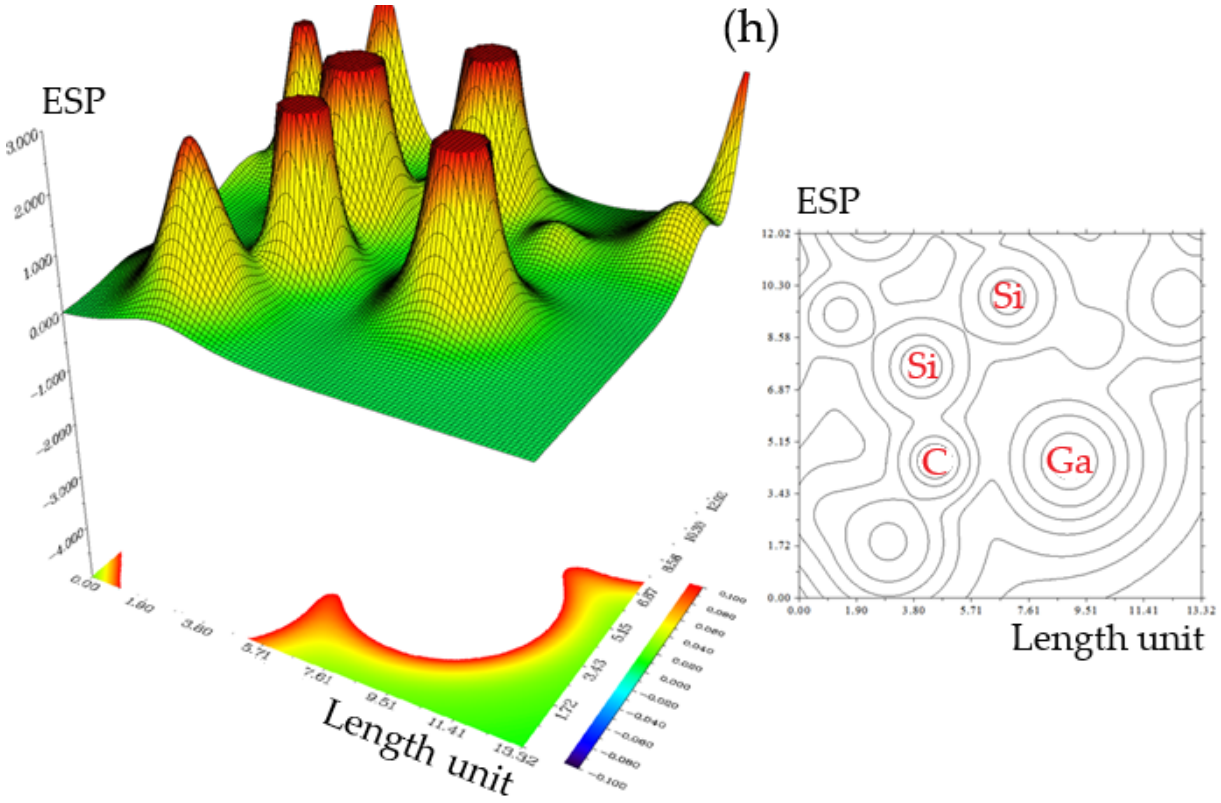

(h)
ESP
Length unit
ESP
Si
Si
C
Ga
Length unit

Figure S2. The shaded (left side) and counter (right side) maps of ESP graphs versus length unit (Bohr) for (a) SiLiC, (b) SiNaC, (c) SiKC, (d) SiBeC, (e) SiMgC, (f) SiBC, (g) SiAlC, (h) SiGaC nanoclusters.

Table S1. The atomic charge (Q/coulomb) for SiLiC, SiNaC, SiKC, SiBeC, SiMgC, SiBC, SiAlC, SiGaC nanoclusters.

SiLiC		SiNaC		SiKC		SiBeC	
Atom	Q	Atom	Q	Atom	Q	Atom	Q
Si(1)	0.76	Si(1)	0.74	Si(1)	0.75	Si(1)	0.74
C(2)	–0.42	C(2)	–0.42	C(2)	–0.43	C(2)	–0.43
C(3)	–0.34	C(3)	–0.37	C(3)	–0.34	C(3)	–0.36
Si(4)	0.73	Si(4)	0.73	Si(4)	0.73	Si(4)	0.74
Si(5)	0.73	Si(5)	0.74	Si(5)	0.75	Si(5)	0.72
Si(6)	0.79	Si(6)	0.85	Si(6)	0.83	Si(6)	0.82
C(7)	–0.38	C(7)	–0.40	C(7)	–0.39	C(7)	–0.39
C(8)	–0.36	C(8)	–0.37	C(8)	–0.37	C(8)	–0.34
C(9)	–0.38	C(9)	–0.37	C(9)	–0.37	C(9)	–0.38
C(10)	–0.81	C(10)	–0.70	C(10)	–1.01	C(10)	–0.83
C(11)	–0.37	C(11)	–0.35	C(11)	–0.32	C(11)	–0.38
C(12)	–0.92	C(12)	–0.82	C(12)	–0.90	C(12)	–0.89
Si(13)	1.11	Si(13)	0.96	Si(13)	0.99	Si(13)	1.05
C(14)	–0.37	C(14)	–0.37	C(14)	–0.36	C(14)	–0.36
C(15)	–0.38	C(15)	–0.38	C(15)	–0.41	C(15)	–0.34
Si(16)	0.81	Si(16)	0.86	Si(16)	0.86	Si(16)	0.83
C(17)	–0.41	C(17)	–0.42	C(17)	–0.43	C(17)	–0.41
C(18)	–0.35	C(18)	–0.37	C(18)	–0.38	C(18)	–0.34
Si(19)	0.71	Si(19)	0.71	Si(19)	0.70	Si(19)	0.70
Si(20)	0.75	Si(20)	0.77	Si(20)	0.74	Si(20)	0.75
Si(21)	0.76	Si(21)	0.75	Si(21)	0.75	Si(21)	0.74
C(22)	–0.38	C(22)	–0.40	C(22)	–0.40	C(22)	–0.39
C(23)	–0.34	C(23)	–0.38	C(23)	–0.36	C(23)	–0.36
C(24)	–0.78	C(24)	–0.69	C(24)	–0.96	C(24)	–0.86
C(25)	–0.34	C(25)	–0.34	C(25)	–0.32	C(25)	–0.35
C(26)	–0.85	C(26)	–0.75	C(26)	–0.91	C(26)	–0.82
C(27)	–0.51	C(27)	–0.47	C(27)	–0.46	C(27)	–0.49
Si(28)	1.07	Si(28)	1.01	Si(28)	1.04	Si(28)	1.05
C(29)	–0.40	C(29)	–0.39	C(29)	–0.42	C(29)	–0.37
C(30)	–0.37	C(30)	–0.39	C(30)	–0.37	C(30)	–0.34
Li(31)	0.75	Na(31)	0.68	K(31)	0.91	Be(31)	0.65
Li(32)	0.50	Na(32)	0.37	K(32)	0.90	Be(32)	0.67
SiMgC		SiBC		SiAlC		SiGaC	
Atom	Q	Atom	Q	Atom	Q	Atom	Q
Si(1)	0.73	Si(1)	0.77	Si(1)	0.76	Si(1)	0.76
C(2)	–0.43	C(2)	–0.42	C(2)	–0.42	C(2)	–0.42
C(3)	–0.34	C(3)	–0.34	C(3)	–0.33	C(3)	–0.33
Si(4)	0.72	Si(4)	0.75	Si(4)	0.76	Si(4)	0.76
Si(5)	0.71	Si(5)	0.75	Si(5)	0.74	Si(5)	0.74
Si(6)	0.81	Si(6)	0.83	Si(6)	0.87	Si(6)	0.86
C(7)	–0.39	C(7)	–0.38	C(7)	–0.39	C(7)	–0.39
C(8)	–0.34	C(8)	–0.36	C(8)	–0.34	C(8)	–0.34
C(9)	–0.35	C(9)	–0.38	C(9)	–0.34	C(9)	–0.35
C(10)	–1.07	C(10)	–0.76	C(10)	–1.23	C(10)	–1.14

C(11)	–0.37	C(11)	–0.36	C(11)	–0.33	C(11)	–0.34
C(12)	–1.10	C(12)	–0.81	C(12)	–1.08	C(12)	–1.01
Si(13)	1.09	Si(13)	1.06	Si(13)	1.06	Si(13)	1.10
C(14)	–0.38	C(14)	–0.33	C(14)	–0.35	C(14)	–0.34
C(15)	–0.38	C(15)	–0.34	C(15)	–0.35	C(15)	–0.35
Si(16)	0.83	Si(16)	0.84	Si(16)	0.88	Si(16)	0.87
C(17)	–0.42	C(17)	–0.43	C(17)	–0.43	C(17)	–0.43
C(18)	–0.34	C(18)	–0.36	C(18)	–0.35	C(18)	–0.34
Si(19)	0.69	Si(19)	0.72	Si(19)	0.69	Si(19)	0.69
Si(20)	0.75	Si(20)	0.78	Si(20)	0.80	Si(20)	0.80
Si(21)	0.73	Si(21)	0.77	Si(21)	0.75	Si(21)	0.75
C(22)	–0.39	C(22)	–0.38	C(22)	–0.38	C(22)	–0.38
C(23)	–0.35	C(23)	–0.35	C(23)	–0.33	C(23)	–0.33
C(24)	–1.05	C(24)	–0.77	C(24)	–1.20	C(24)	–1.10
C(25)	–0.32	C(25)	–0.35	C(25)	–0.33	C(25)	–0.34
C(26)	–1.06	C(26)	–0.76	C(26)	–1.07	C(26)	–1.00
C(27)	–0.48	C(27)	–0.45	C(27)	–0.41	C(27)	–0.42
Si(28)	1.08	Si(28)	1.01	Si(28)	1.04	Si(28)	1.05
C(29)	–0.42	C(29)	–0.30	C(29)	–0.34	C(29)	–0.33
C(30)	–0.37	C(30)	–0.34	C(30)	–0.36	C(30)	–0.35
Mg(31)	1.15	B(31)	0.40	Al(31)	0.93	Ga(31)	0.76
Mg(32)	1.09	B(32)	0.32	Al(32)	1.13	Ga(32)	0.92

Table S2. The bond order of Mayer, Wiberg, Mulliken and Laplacian from mixed alpha and beta density matrix for SiLiC, SiNaC, SiKC, SiBeC, SiMgC, SiBC, SiAlC, SiGaC nanoclusters.

Heteroclusters	Bond type	Bond order			
		Mayer	Wiberg	Mulliken	Laplacian
SiLiC	Si(13)–Si(28)	0.73	0.67	0.56	2.11
	C(10)–Li(32)	0.40	0.42	0.48	0.43
	C(12)–Li(31)	0.16	0.26	0.27	0.27
	C(24)–Li(32)	0.36	0.41	0.44	0.42
	C(26)–Li(31)	0.20	0.31	0.31	0.40
SiNaC	Si(13)–Si(28)	0.69	0.66	0.42	0.47
	C(10)–Na(32)	0.41	0.27	0.59	0.59
	C(12)–Na(31)	0.16	0.20	0.32	0.31
	C(24)–Na(32)	0.41	0.27	0.56	0.53
	C(26)–Na(31)	0.22	0.23	0.37	0.36
SiKC	Si(13)–Si(28)	0.76	0.66	0.97	0.93
	C(10)–K(32)	0.57	0.39	0.54	0.53
	C(12)–K(31)	0.24	0.23	0.11	0.10
	C(24)–K(32)	0.58	0.38	0.42	0.40
	C(26)–K(31)	0.36	0.29	0.20	0.19
SiBeC	Si(13)–Si(28)	0.81	0.69	0.60	0.66
	C(10)–Be(32)	0.82	0.80	0.83	0.85
	C(12)–Be(31)	0.47	0.50	0.42	0.46
	C(24)–Be(32)	0.78	0.77	0.82	0.83
	C(26)–Be(31)	0.59	0.62	0.50	0.52
SiMgC	Si(13)–Si(28)	0.89	0.69	0.68	0.63
	C(10)–Mg(32)	0.56	0.62	0.63	0.60

	C(12)–Mg(31)	0.33	0.44	0.40	0.44
	C(24)–Mg(32)	0.54	0.60	0.60	0.61
	C(26)–Mg(31)	0.41	0.52	0.45	0.47
SiBC	Si(13)–Si(28)	0.81	0.70	0.25	2.12
	C(10)–B(32)	0.86	0.95	0.55	0.19
	C(12)–B(31)	0.36	0.53	0.62	0.95
	C(24)–B(32)	0.90	0.96	0.57	0.15
	C(26)–B(31)	0.44	0.64	0.75	0.80
SiAlC	Si(13)–Si(28)	0.97	0.70	0.40	0.72
	C(10)–Al(32)	0.69	0.84	0.44	0.46
	C(12)–Al(31)	0.30	0.48	0.49	0.42
	C(24)–Al(32)	0.71	0.83	0.53	0.38
	C(26)–Al(31)	0.38	0.60	0.50	0.50
SiGaC	Si(13)–Si(28)	0.88	0.70	0.52	0.65
	C(10)–Ga(32)	0.80	0.87	0.47	0.58
	C(12)–Ga(31)	0.33	0.48	0.46	0.65
	C(24)–Ga(32)	0.81	0.86	0.52	0.48
	C(26)–Ga(31)	0.41	0.61	0.70	0.63