Supplementary Information

The 4*d* and 5*d* Bimetal Doped Tubular Silicon Clusters M_2Si_{12} with M = Nb, Ta, Mo and W: A Bimetallic Configuration Model

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Contents

Table S1. the relative energy (kcal/mol) of lower-lying spin state of dimers. M: multiplicity.

Figure S1. The shape of lower-lying isomer of Nb_2Si_{12}, $Nb_2Si_{12}^{2-}$, Ta_2Si_{12} and $Ta_2Si_{12}^{2-}$ clusters. The geometry optimizations were performed using the BP86/aug-cc-pVTZ:M; 6-311+g(d):Si level of theory.

Figure S2. The shape of lower-lying isomer of Mo_2Si_{12}, $Mo_2Si_{12}^{2+}$, W_2Si_{12} and $W_2Si_{12}^{2+}$ clusters. The geometry optimizations were performed using the BP86/aug-cc-pVTZ:M; 6-311+g(d):Si level of theory.

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Figure S3. The shape of lower-lying isomer of Mo_2Si_{12}, $Mo_2Si_{12}^{2+}$, W_2Si_{12} and $W_2Si_{12}^{2+}$ clusters. The geometry optimizations were performed using the BP86/aug-cc-pVTZ:M; 6-311+g(d):Si level of theory.

Figure S4. The DOS and pDOS of $Si_{12}Nb_2$ cluster.

Figure S5. The DOS and pDOS of $Si_{12}NbMo$ cluster.

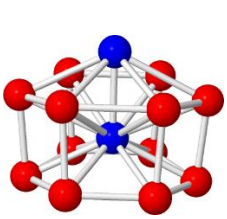
Figure S6. The DOS and pDOS of $Si_{12}Ta_2$ cluster.

Figure S7. The DOS and pDOS of $Si_{12}W_2$ cluster.

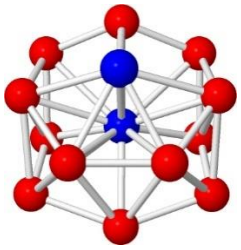
Figure S8. The DOS and pDOS of $Si_{12}TaW$ cluster.

Table S1.

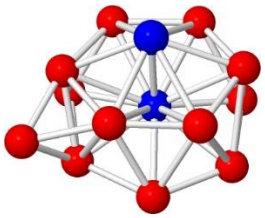
Specie	M=1	M=3	M=5	M=7	Specie	M=2	M=4	M=6	M=8
Mo_2	0.0	25.0	40.0	55.6	MoNb	0.0	21.9	42.7	73.3
Nb_2	8.4	0.0	22.0	49.2	WTa	2.2	0.0	22.8	49.4
W_2	0.0	7.8	19.6	36.4					
Ta_2	30.7	2.0	0.0	27.1					



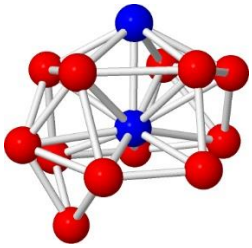
Nb2.A
C_{2v} $^1A_1$ 0.00
C_{6v} $^3A_1$ 9.37



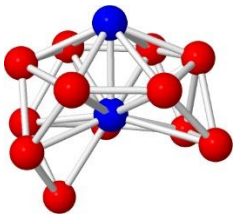
Nb2.B
C_s ^{1}A’ 20.89
C_1 ^{3}A 23.12



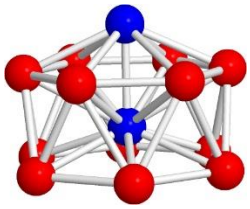
Nb2.C
C_1 ^{1}A 19.72
C_1 ^{3}A 31.78
Nb_2Si_{12}



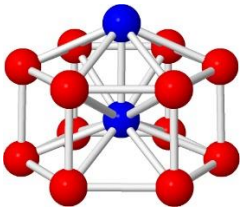
Nb2.D
C_1 ^{1}A 20.80
C_1 ^{3}A 28.39



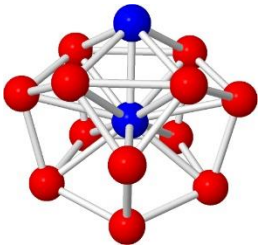
Nb2.E
C_1 ^{1}A 15.42
C_1 ^{3}A 23.12



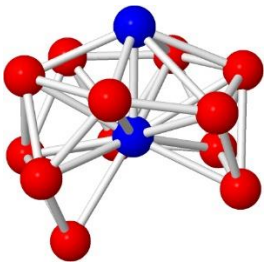
Nb2.da.A
C_{6v} $^1A_1$ 0.00



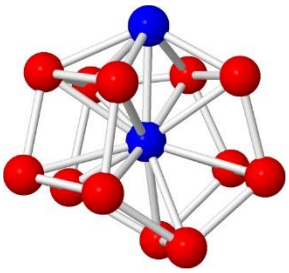
Nb2.da.B
C_{6v} $^1A_1$ 26.9



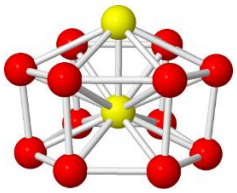
Nb2.da.C
C_s ^{1}A’ 28.04
$Si_{12}Nb_2^{2-}$



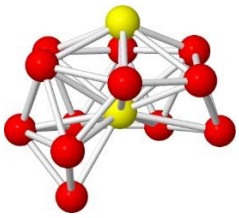
Nb2.da.D
C_1 ^{1}A 28.51



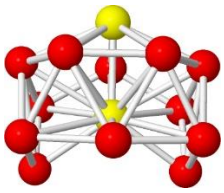
Nb2.da.E
C_1 ^{1}A 32.95



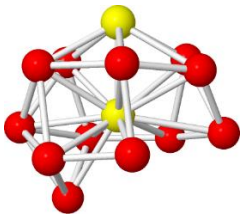
Ta2.A
C_{2v} $^1A_1$ 0.00
C_6 ^{3}A 10.69



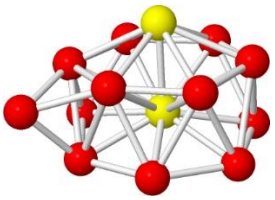
Ta2.B
C_1 ^{1}A 14.59
C_1 ^{3}A 21.92



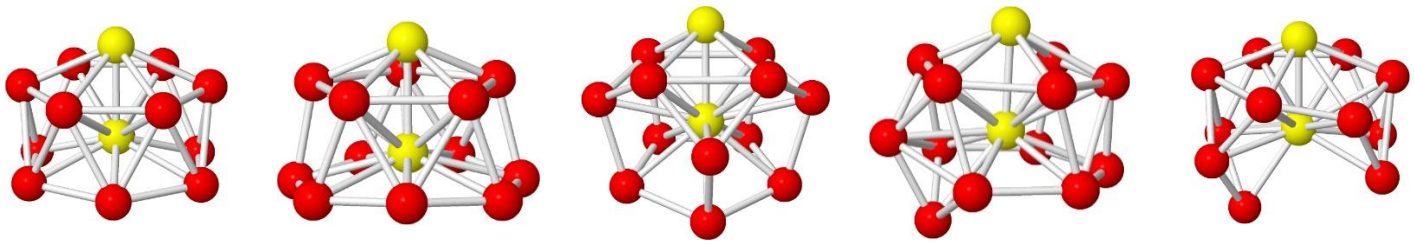
Ta2.C
C_s ^{1}A’ 18.40
C_1 ^{3}A 21.92
Ta_2Si_{12}



Ta2.D
C_1 ^{1}A 18.51
C_1 ^{3}A 19.55



Ta2.E
C_1 ^{1}A 20.75
C_1 ^{3}A 33.12



Ta2.da.A
C_{6v} $^1A_1$ 0.00

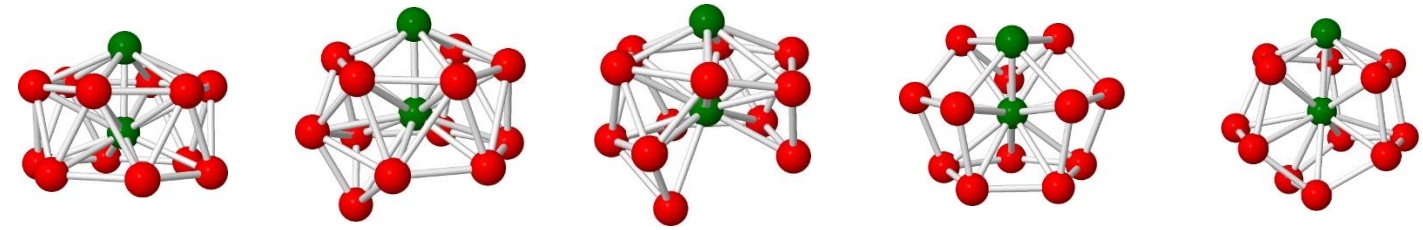
Ta2.da.B
C_s ^{1}A'10.39

Ta2.da.C
C_s ^{1}A'24.15
$Si_{12}Ta_2^{2-}$

Ta2.da.D
C_1 ^{1}A 23.86

Ta2.da.E
C_1 ^{1}A 25.59

Figure S1.



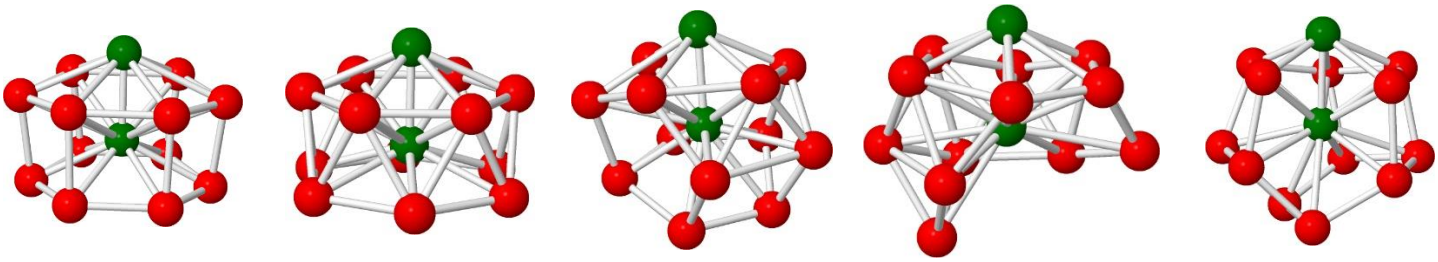
Mo2.A
C_{6v} $^1A_1$ 0.00
C_{2v} $^3A_1$ 28.07

Mo2.B
C_1 ^{1}A 26.60
C_1 ^{3}A 30.44

Mo2.C
C_1 ^{1}A 36.23
C_1 ^{3}A 42.19
Mo_2Si_{12}

Mo2.D
C_s ^{1}A' 30.20
C_s ^{3}A' 44.60

Mo2.E
C_1 ^{1}A 36.89
C_1 ^{3}A 42.70



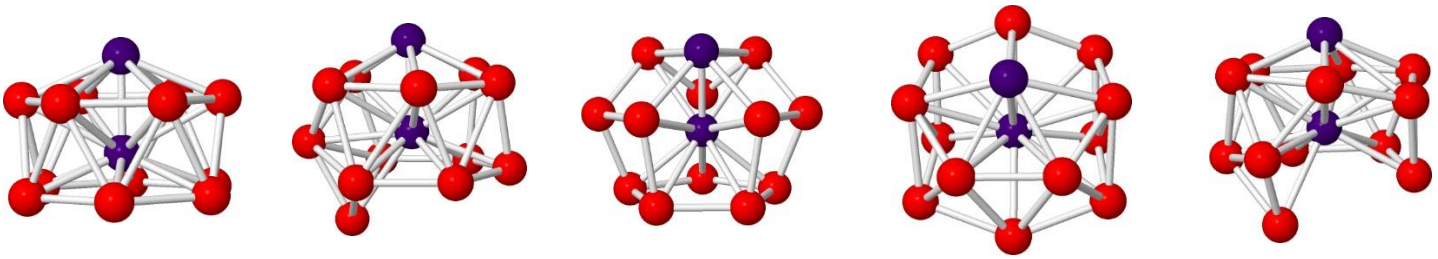
Si12Mo2-dica_2
C_{2v} $^1A_1$ 0.00

Si12Mo2-dica_1
C_{6v} $^1A_1$ 6.85

Si12Mo2-dica_3
C_1 ^{1}A 22.42
$Mo_2Si_{12}^{2+}$

Si12Mo2-dica_4
C_1 ^{1}A 24.92

Si12Mo2-dica_5
C_1 ^{1}A 25.50



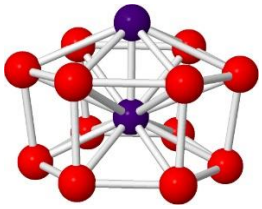
W2.n.A
C_{6v} $^1A_1$ 0.00
C_{2v} $^3A_1$ 32.78

W2.B
C_1 ^{1}A 24.26
C_1 ^{3}A 32.19

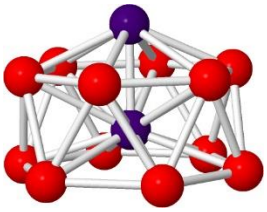
W2.C
C_s ^{1}A' 28.24
C_s ^{3}A' 43.82
W_2Si_{12}

W2.D
C_s ^{1}A' 33.28
C_s ^{3}A' 50.42

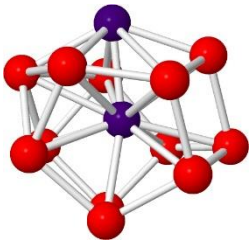
W2.E
C_1 ^{1}A 34.68
C_1 ^{3}A 41.19



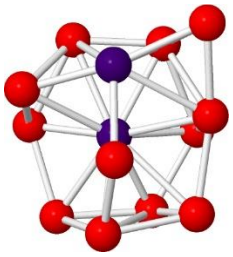
Si12W2-dica_2
C_{2v} $^1A_1$ 0.00



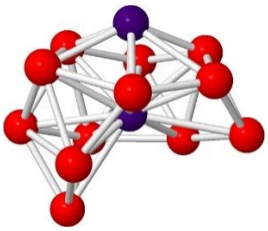
Si12W2-dica_1
C_{6v} $^1A_1$ 16.68



Si12W2-dica_3
C_1 ^1A 23.86



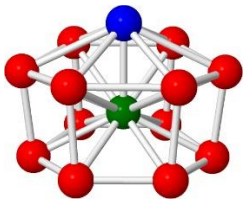
Si12W2-dica_8
C_1 ^1A 23.38



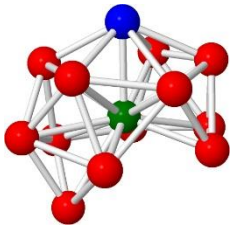
Si12W2-dica_6
C_1 ^1A 25.38

$Si_{12}W_2^{2+}$

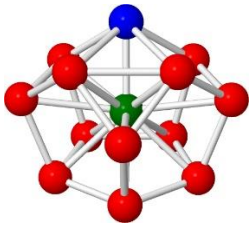
Figure S2



NbMo.c.A
C_{2v} $^1A_1$ 0.00

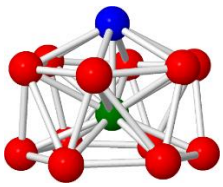


NbMo.c.B
C_1 ^1A 25.00

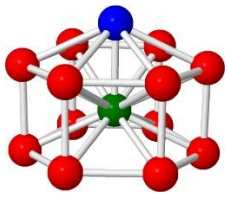


NbMo.c.C
C_s $^1A'$ 28.23

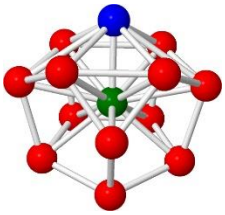
$NbMoSi_{12}^+$



NbMo.a.A
C_{6v} $^1A_1$ 0.00



NbMo.a.B
C_{6v} $^1A_1$ 22.84



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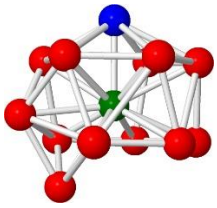

NbMo.a.D
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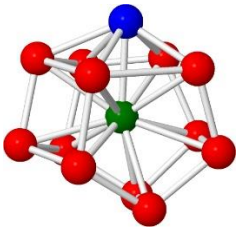
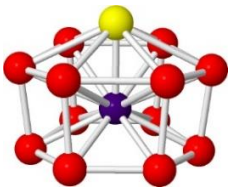
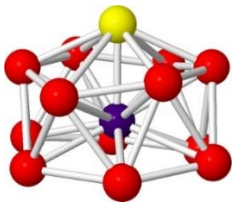
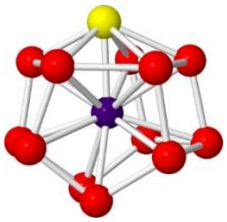


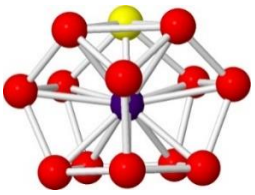
NbMo.a.E
C_1 ^1A 34.24

$NbMoSi_{12}^-$



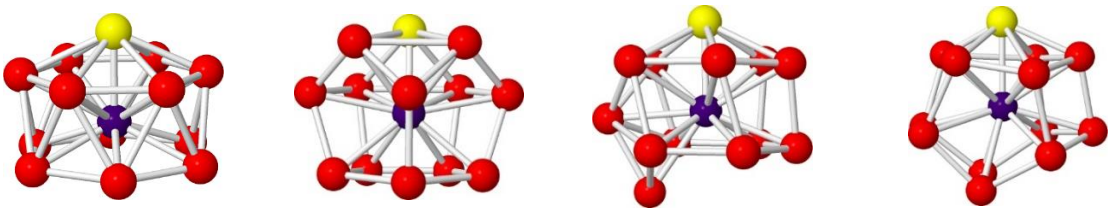






TaW.c.A	TaW.c.B	TaW.c.C	TaW.c.D
C_{2v} $^1A_1$ 0.00	C_{2v} $^1A_1$ 14.22	C_1 ^1A 23.98	C_s $^1A'$ 26.65

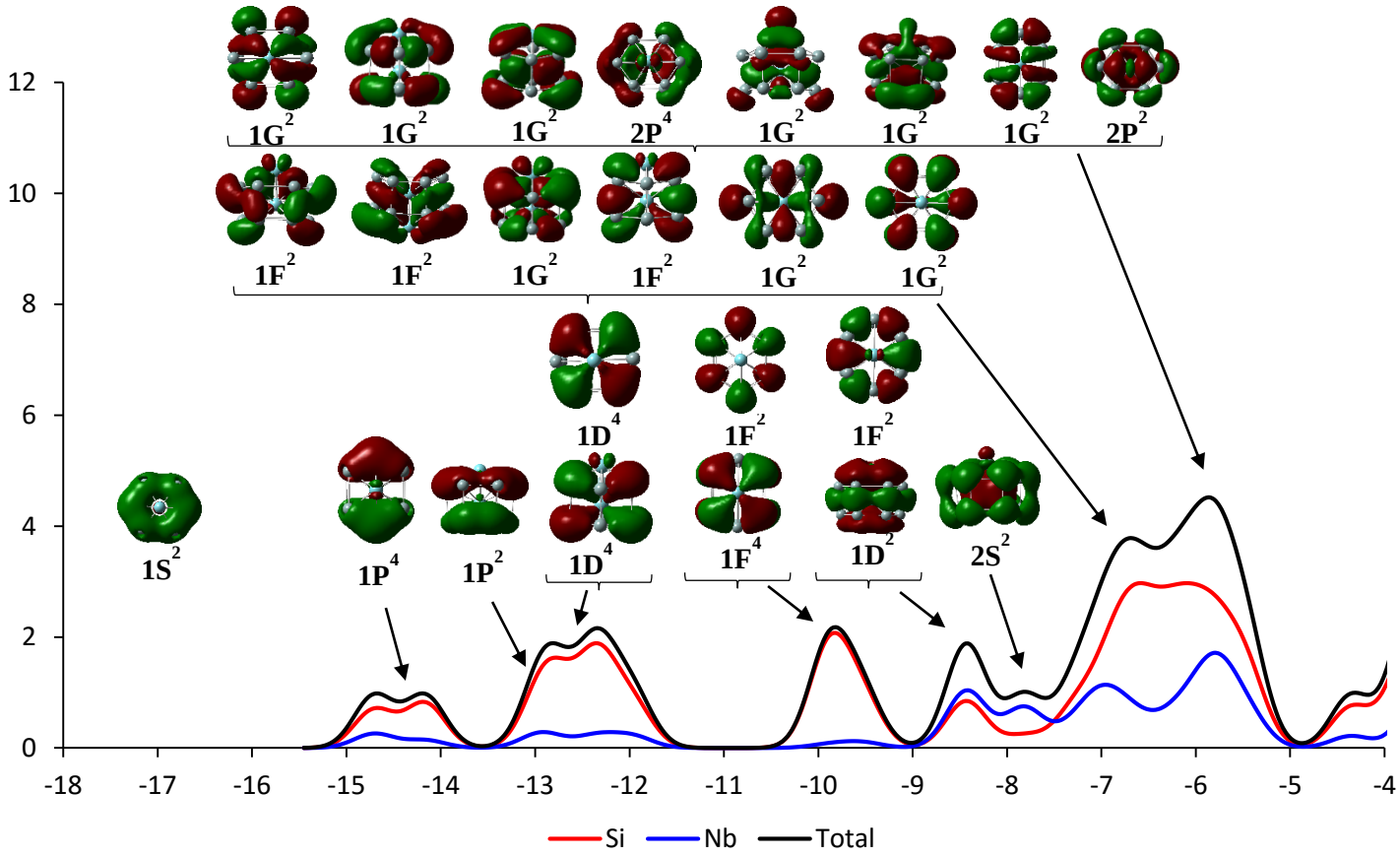
$TaWSi_{12}^+$



TaW.a.A	TaW.a.B	TaW.a.C	TaW.a.D
C_{6v} $^1A_1$ 0.00	C_s $^1A'$ 22.25	C_1 ^1A 24.42	C_1 ^1A 31.54

$TaWSi_{12}^-$

Figure S3



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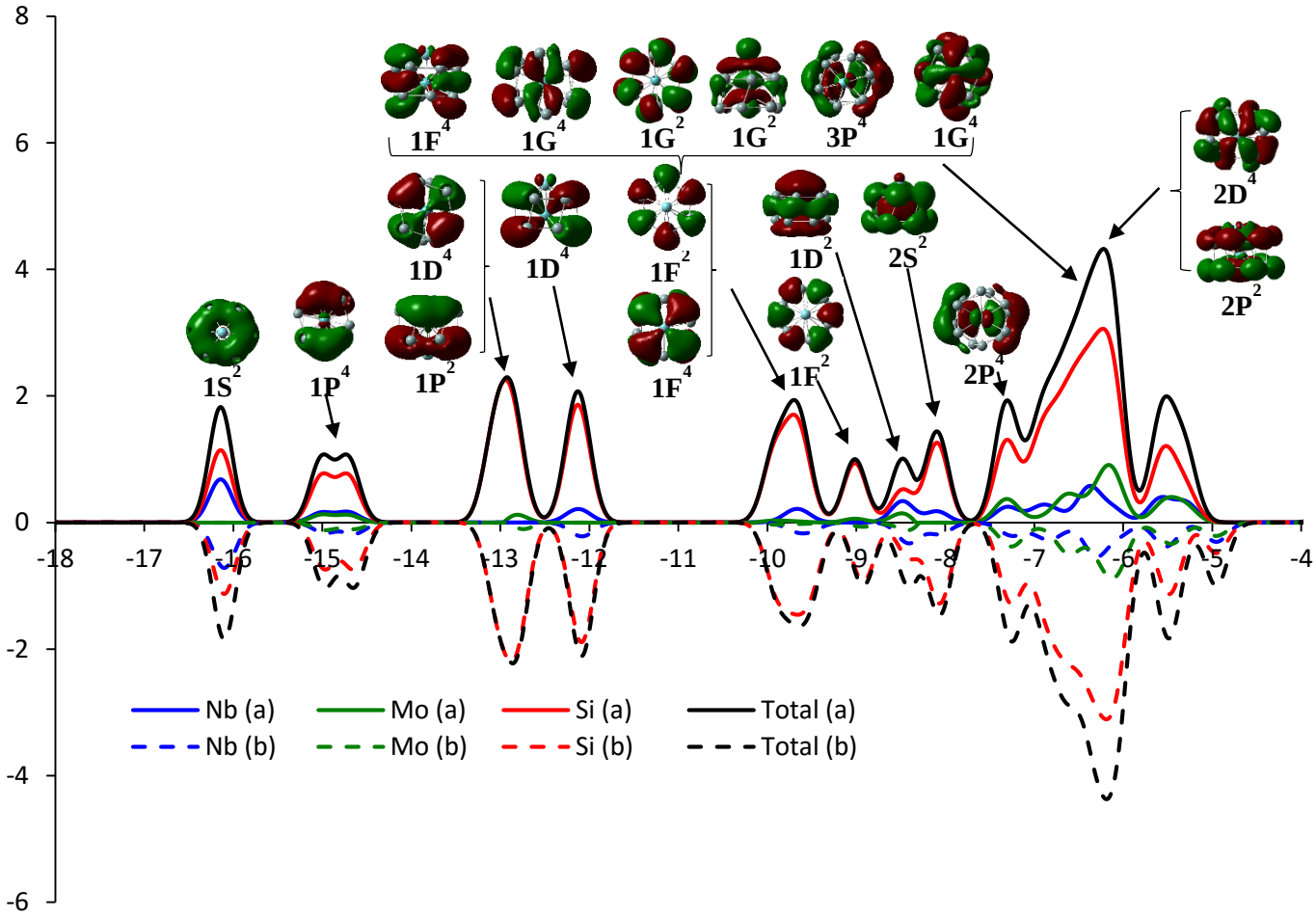
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1G2
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1G4
2D4
2P2
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1F2
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Mo (a)
Si (a)
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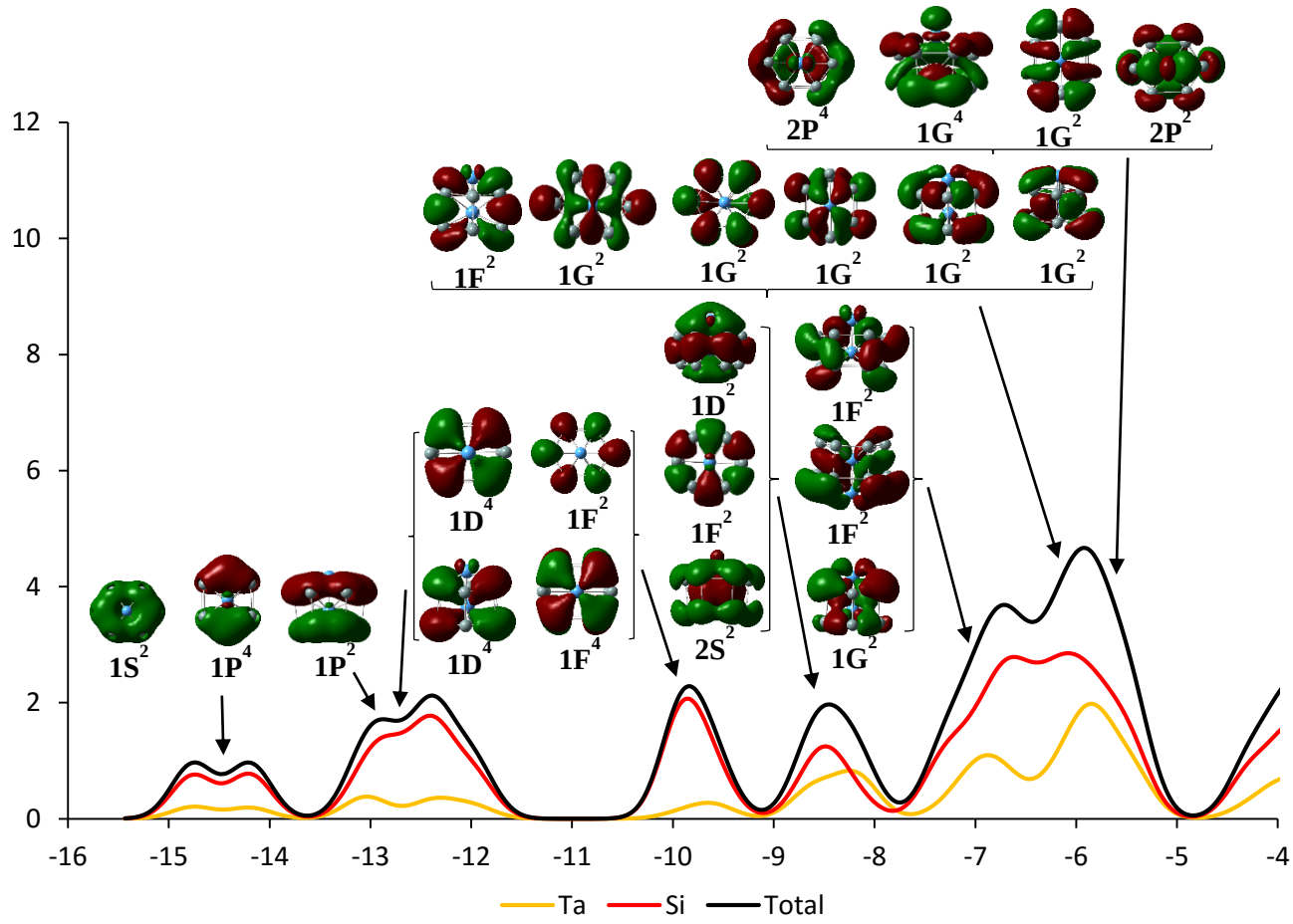
Nb (b)
Mo (b)
Si (b)
Total (b)

Figure S5.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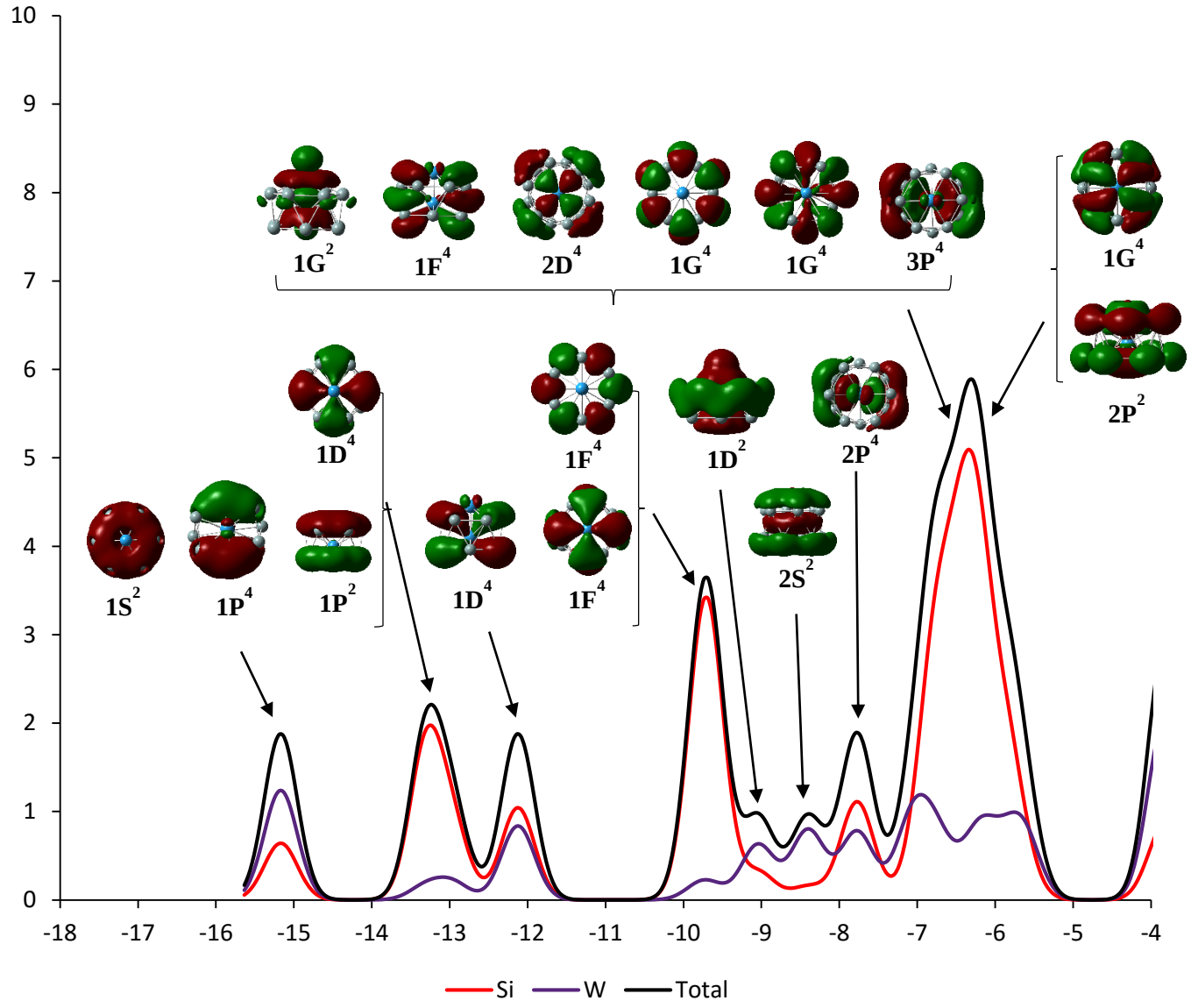
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1
0
-18
-17
-16
-15
-14
-13
-12
-11
-10
-9
-8
-7
-6
-5
-4
1G2
1F4
2D4
1G4
1G4
3P4
1G4
2P2
1D4
1F4
1D2
2P4
1S2
1P4
1P2
1D4
1F4
2S2
Si
W
Total

Figure S7.

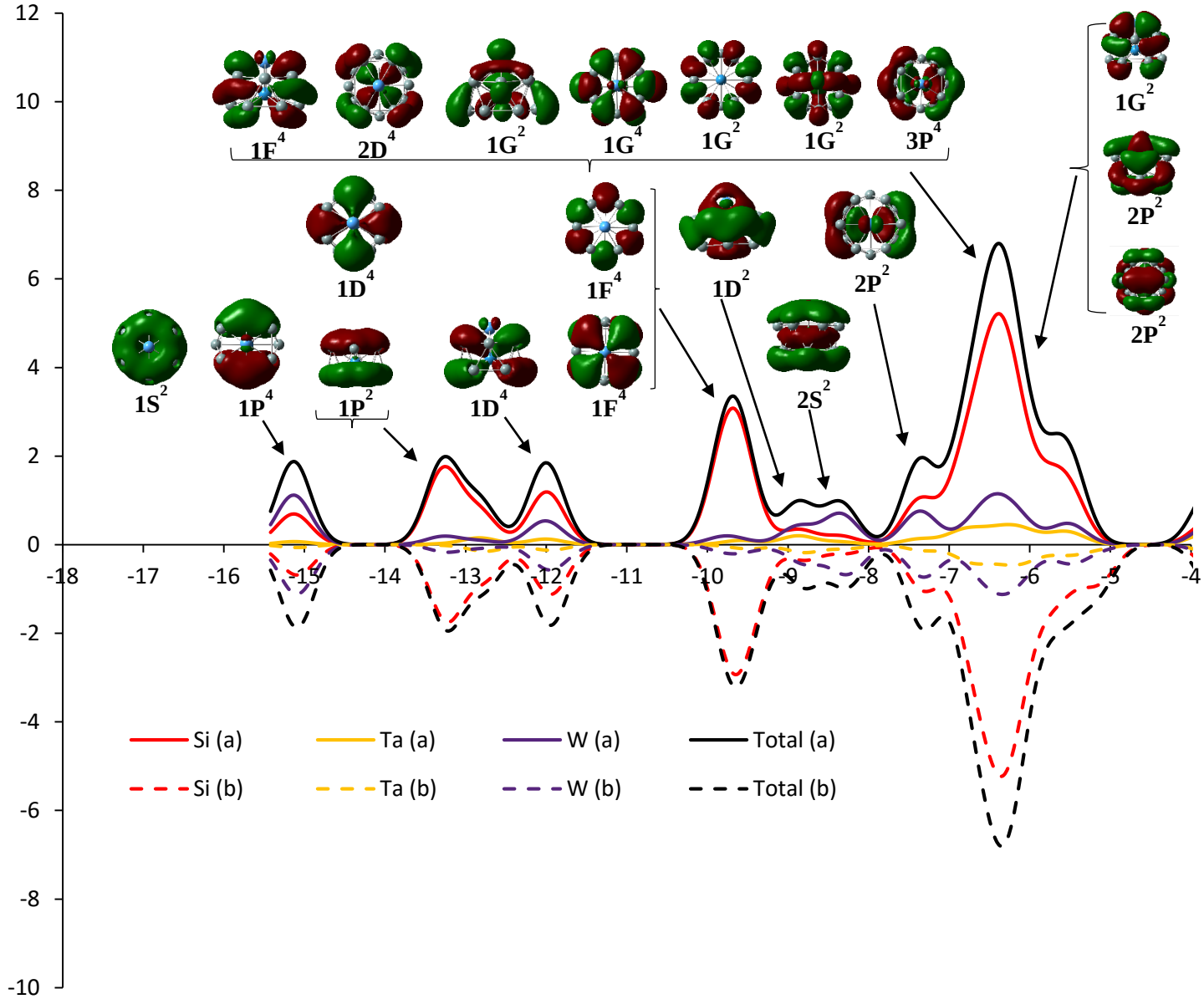
12
10
8
6
4
2
0
-2
-4
-6
-8
-10
-18
-17
-16
-15
-14
-13
-12
-11
-10
-9
-8
-7
-6
-5
-4
1S2
1P4
1P2
1D4
1F4
1F4
1D4
1D2
2S2
2P2
1F4
2D4
1G2
1G4
1G2
1G2
3P4
1G2
2P2
2P2
Si (a)
Ta (a)
W (a)
Total (a)
Si (b)
Ta (b)
W (b)
Total (b)

Figure S8.