

Supporting information for

**Theoretical prediction of superatom WSi<sub>12</sub>-based catalysts for CO  
oxidation by N<sub>2</sub>O**

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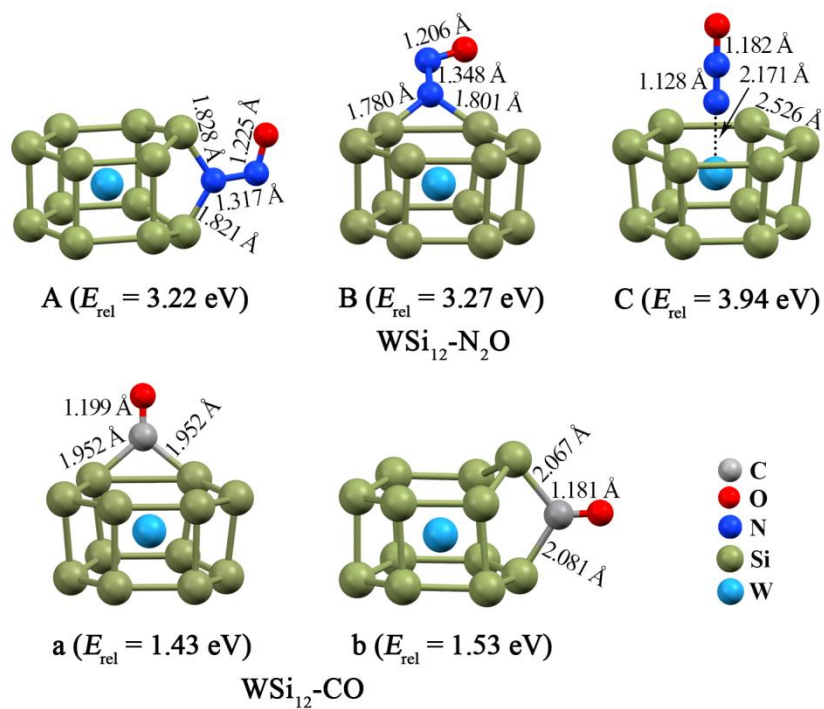
## 1. Table

**Table S1.** The relatively energies (in kcal/mol) of  $\text{MSi}_{12}$  ( $M = \text{Cr, Mo, and W}$ ),  $\text{W}_n\text{Si}_{6(n+1)}$  ( $n = 2, 4, \text{ and } 6$ ),  $\text{MSi}_{12}\text{-N}_2\text{O}$ , and  $\text{W}_n\text{Si}_{6(n+1)}\text{-N}_2\text{O}$  compounds in different spin states at the B3PW91-D3(BJ)/6-311+G(d)&LANL2DZ level.

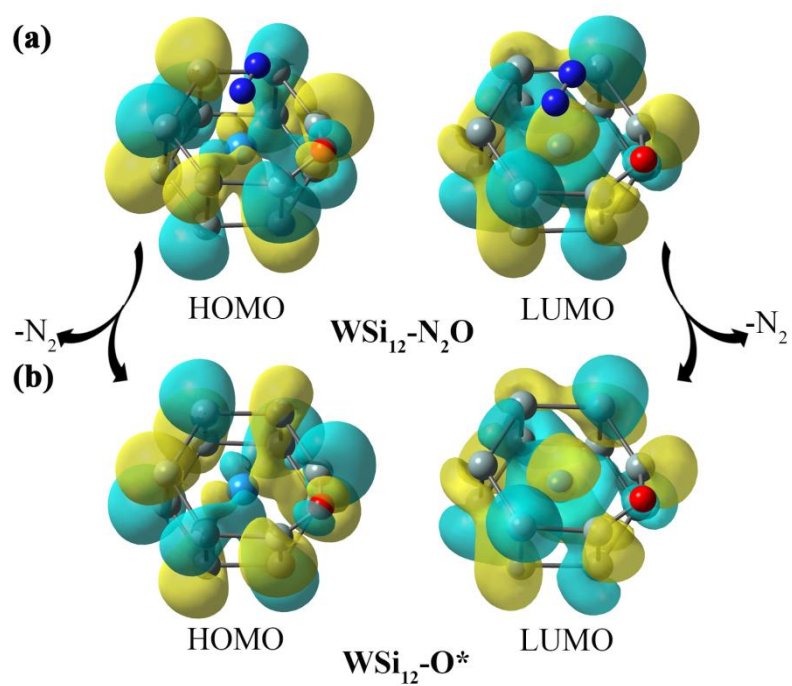
Structures	Singlet	Triplet	Quintet
$\text{CrSi}_{12}$	<b>0.00</b>	5.88	28.43
$\text{MoSi}_{12}$	<b>0.00</b>	23.08	51.92
$\text{WSi}_{12}$	<b>0.00</b>	33.65	48.93
$\text{W}_2\text{Si}_{18}$	<b>0.00</b>	30.08	39.93
$\text{W}_4\text{Si}_{30}$	<b>0.00</b>	21.30	36.14
$\text{W}_6\text{Si}_{42}$	<b>0.00</b>	20.67	22.62
$\text{CrSi}_{12}\text{-N}_2\text{O}$	<b>0.00</b>	3.26	28.75
$\text{MoSi}_{12}\text{-N}_2\text{O}$	<b>0.00</b>	21.04	33.96
$\text{WSi}_{12}\text{-N}_2\text{O}$	<b>0.00</b>	30.74	34.01
$\text{W}_2\text{Si}_{18}\text{-N}_2\text{O}$	<b>0.00</b>	26.38	30.04
$\text{W}_4\text{Si}_{30}\text{-N}_2\text{O}$	<b>0.00</b>	20.84	24.35
$\text{W}_6\text{Si}_{42}\text{-N}_2\text{O}$	<b>0.00</b>	19.69	21.50

## 2. Figures

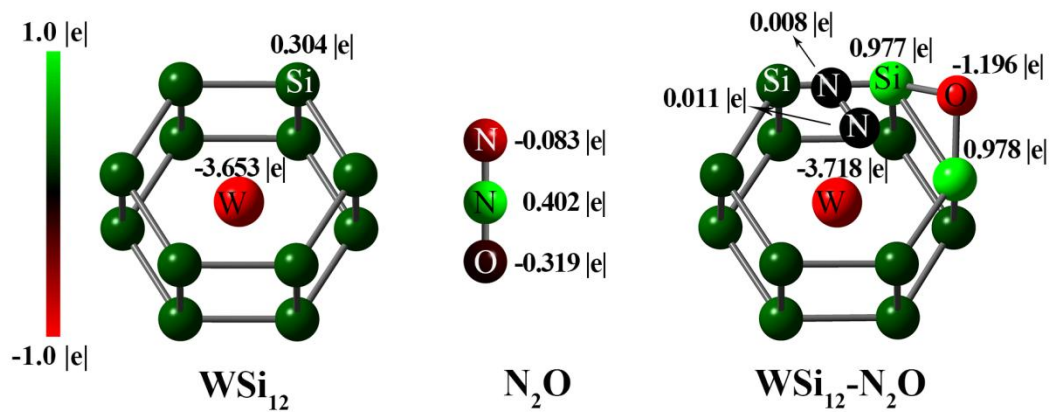
**Figure S1.** Low-lying isomers of  $\text{WSi}_{12}\text{-N}_2\text{O}$  and  $\text{WSi}_{12}\text{-CO}$  with relative energies and selected bond lengths.



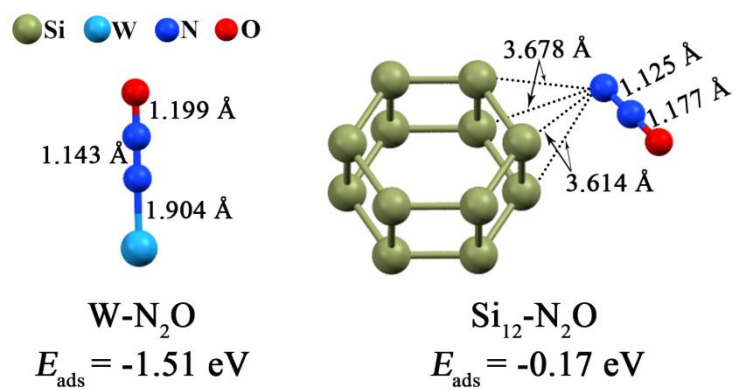
**Figure S2.** The HOMO and LUMO orbitals of (a)  $\text{WSi}_{12}\text{-N}_2\text{O}$  compound and (b)  $\text{WSi}_{12}\text{-O}^*$  intermediate.



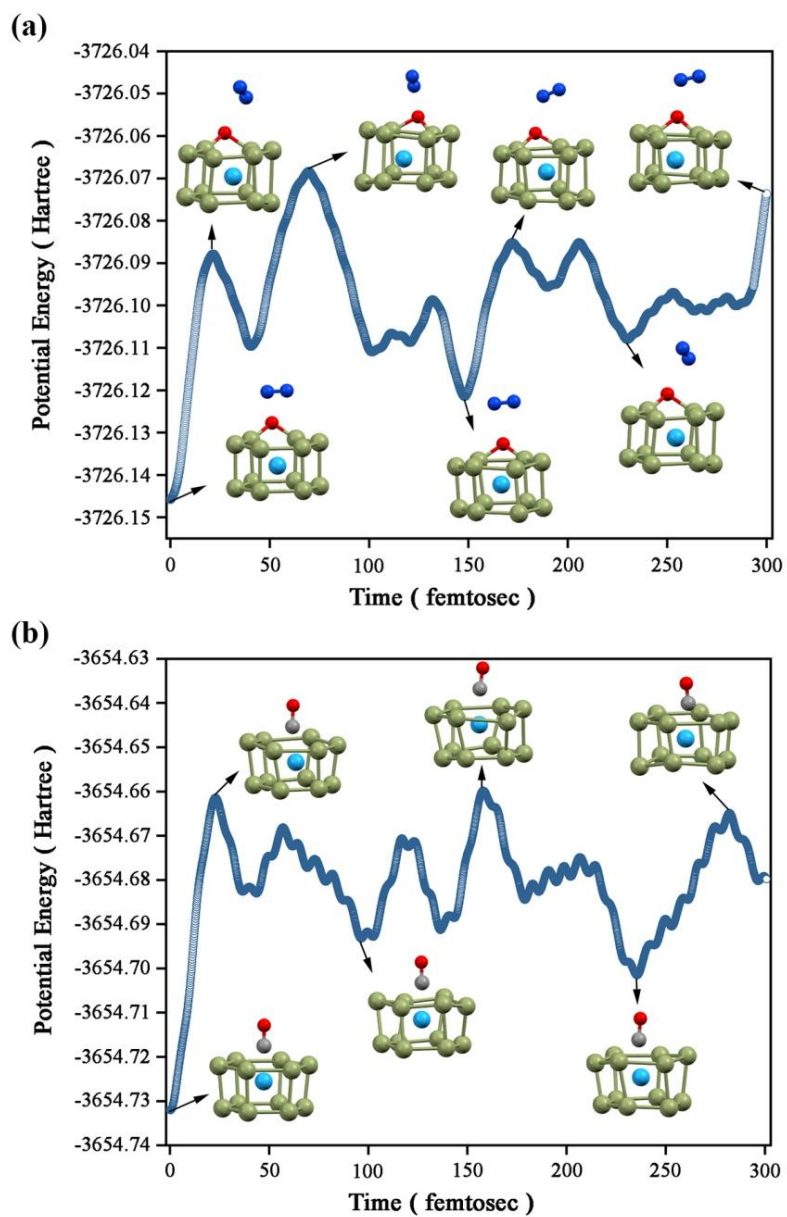
**Figure S3.** The NPA charge distribution of bare  $\text{WSi}_{12}$  superatom, free  $\text{N}_2\text{O}$  molecule, and the most stable  $\text{WSi}_{12}\text{-N}_2\text{O}$  compound.



**Figure S4.** Optimized structures of W-N<sub>2</sub>O and Si<sub>12</sub>-N<sub>2</sub>O compounds, where the Si<sub>12</sub> unit retains its geometric coordinates in the most stable WSi<sub>12</sub> superatom. Selected bond lengths and adsorption energies are also shown.

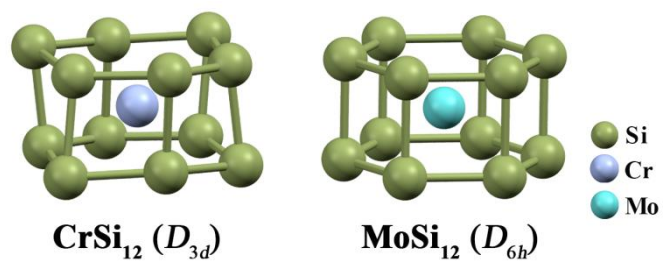


**Figure S5.** Time evolution of the potential energies and structures of (a)  $\text{WSi}_{12}\text{-N}_2\text{O}$  and (b)  $\text{WSi}_{12}\text{-CO}$  during the full length of 300 fs ADMP MD simulation.

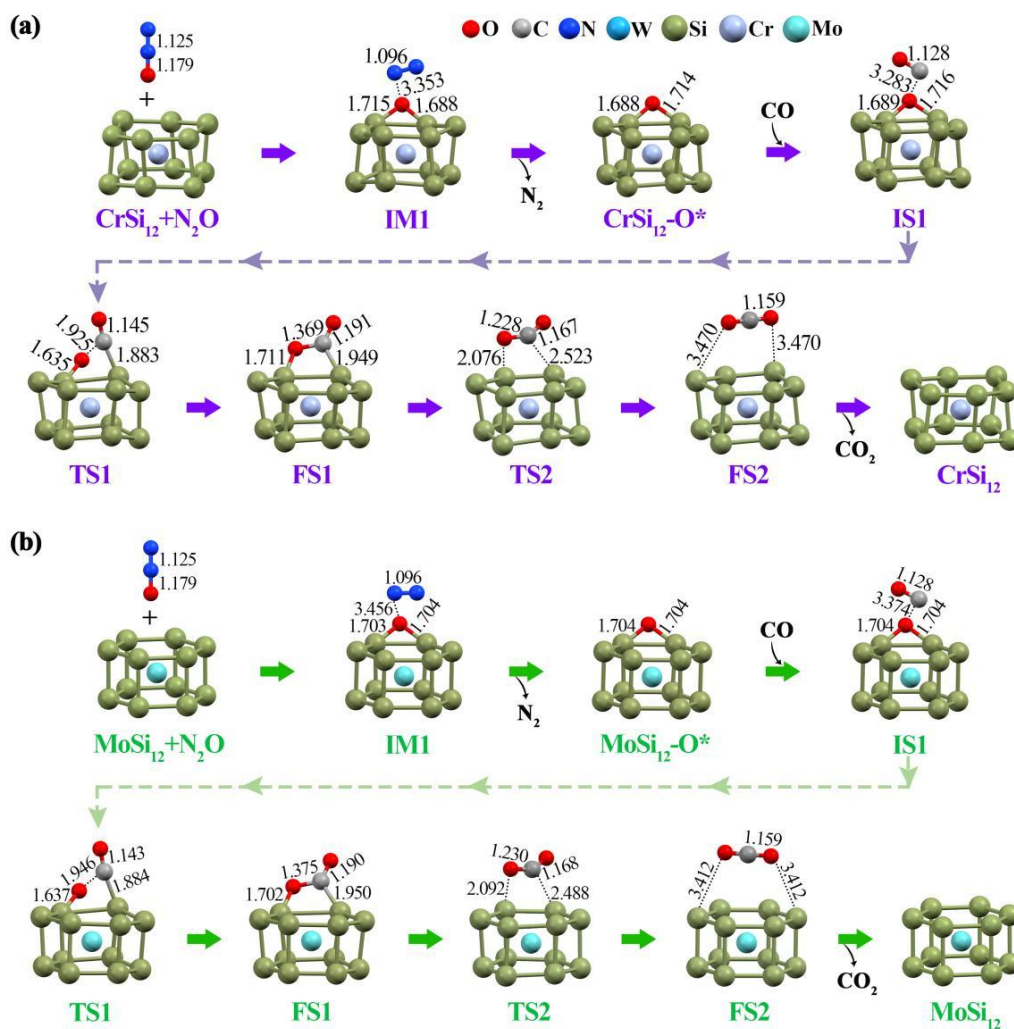




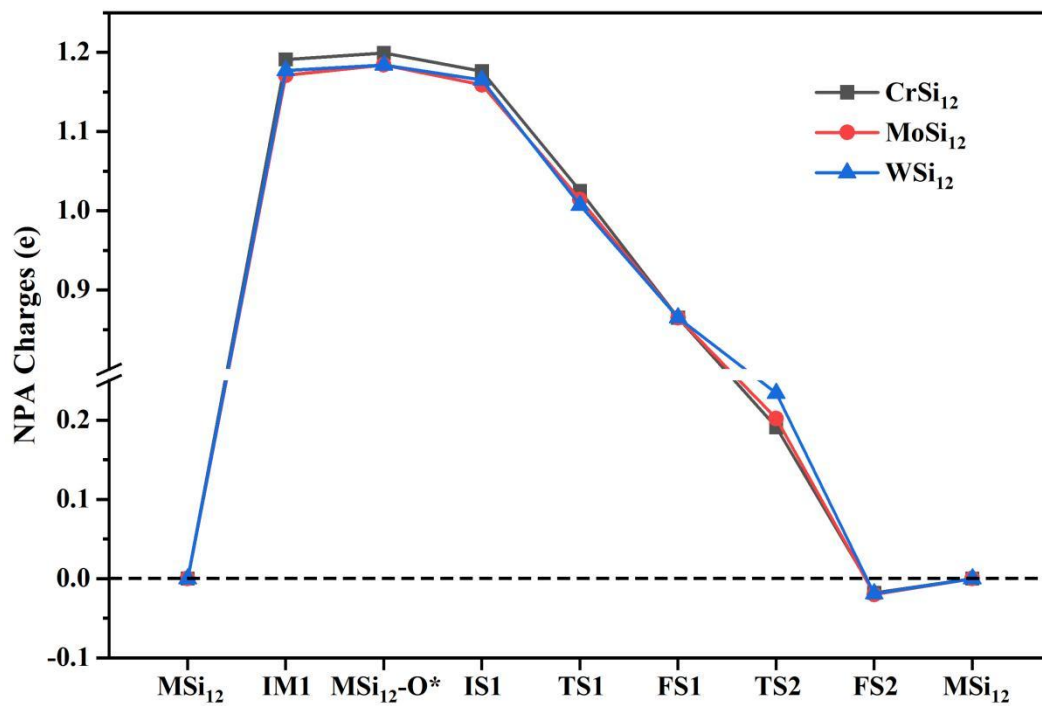
**Figure S6.** The optimized structures of  $\text{CrSi}_{12}$  and  $\text{MoSi}_{12}$  clusters with symmetric group points in the brackets.



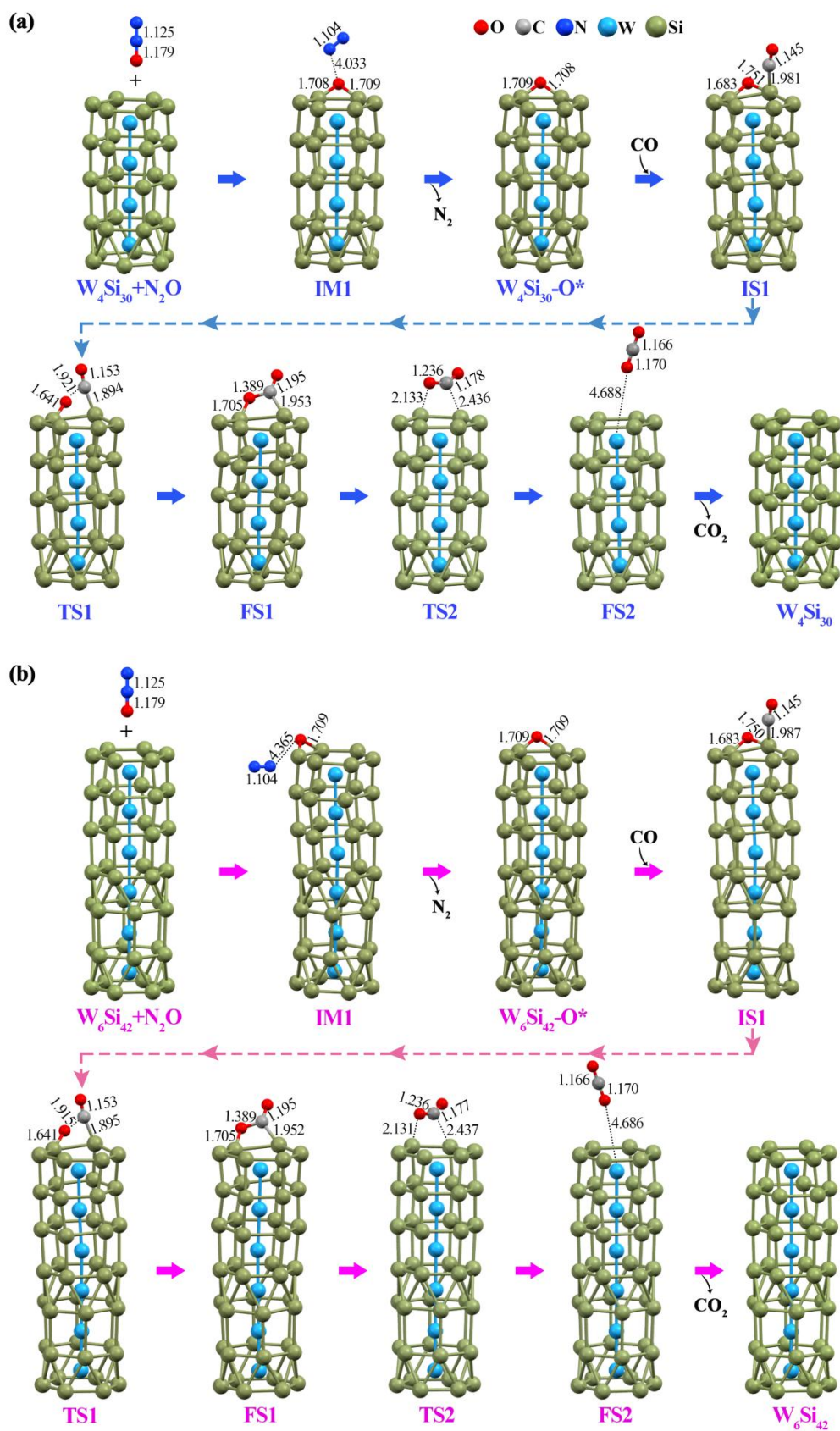
**Figure S7.** Optimized structures of the species involved in the reaction pathway of the CO oxidation by  $N_2O$  reaction on (a)  $CrSi_{12}$  and (b)  $MoSi_{12}$  clusters. Selected bond lengths (in Å) are also shown.



**Figure S8.** The evolution of NPA charges on the  $\text{MSi}_{12}$  ( $M = \text{Cr}, \text{Mo}, \text{and W}$ ) units during the catalytic CO oxidation reaction.

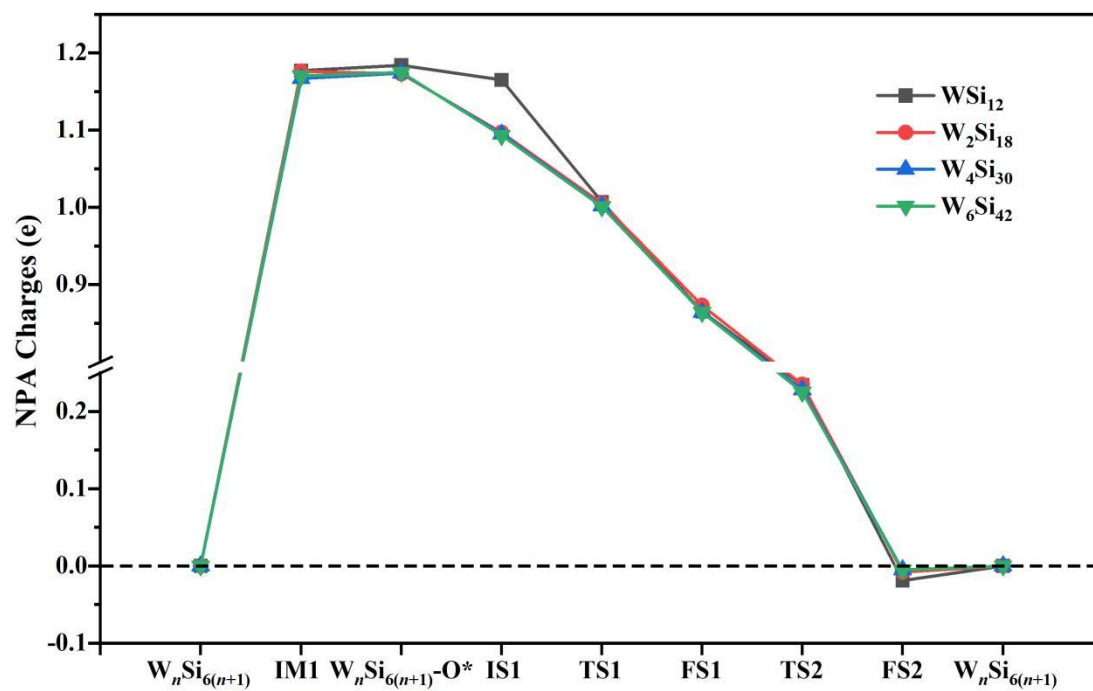


**Figure S9.** Optimized structures of the species involved in the reaction pathways of the CO oxidation by  $N_2O$  reaction on (a)  $W_4Si_{30}$  and (b)  $W_6Si_{42}$  clusters. Selected bond lengths (in Å) are also shown.

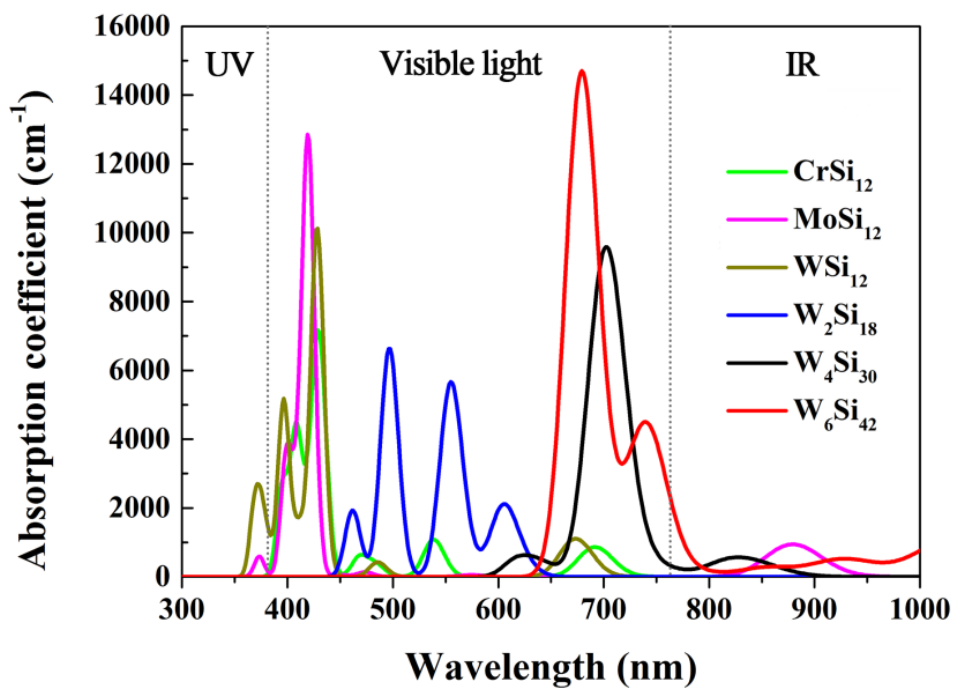




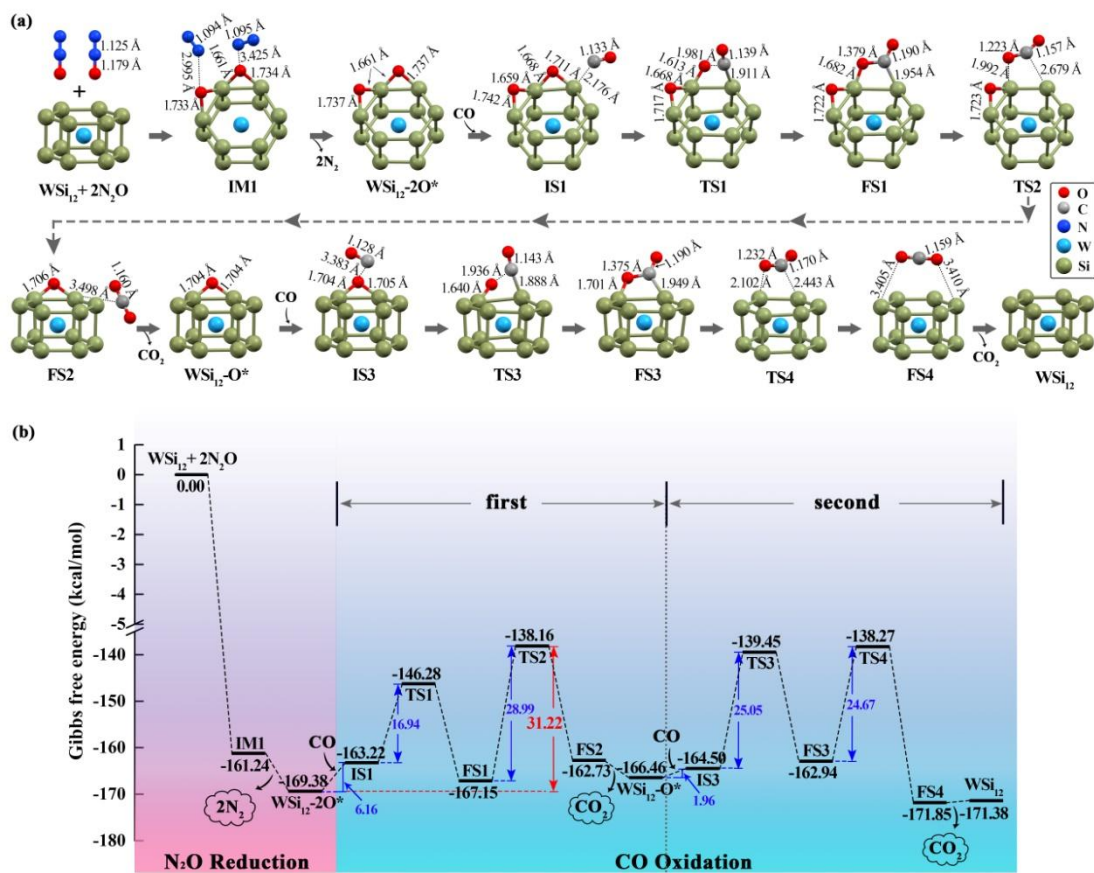
**Figure S10.** The evolution of NPA charges on the  $W_nSi_{6(n+1)}$  ( $n = 2, 4, 6$ ) units during the catalytic CO oxidation reaction.



**Figure S11.** Absorption spectra of  $\text{MSi}_{12}$  ( $\text{M} = \text{Cr}, \text{Mo}, \text{W}$ ) and  $\text{W}_n\text{Si}_{6(n+1)}$  ( $n = 2, 4, 6$ ) clusters. All the optical absorption spectra were reflected under a full-width at half-maximum of 0.05 eV.



**Figure S12.** (a) Optimized structures of the species involved in the reaction pathways of the CO oxidation by two adsorbed N<sub>2</sub>O molecules on WSi<sub>12</sub>. (b) The potential energy profile of the CO oxidation by two adsorbed N<sub>2</sub>O molecules on WSi<sub>12</sub>.





### 3. Cartesian Coordinates

(1)  $\text{MSi}_{12}$  (M = Cr, Mo, and W) and  $\text{W}_n\text{Si}_{6(n+1)}$  ( $n = 2, 4,$  and  $6$ ) clusters

#### **CrSi<sub>12</sub>**

Si	0.00000000	2.20559800	1.08731000
Si	2.14273900	1.23711100	1.28493100
Si	1.91010400	-1.10279900	1.08731000
Si	0.00000000	-2.47422200	1.28493100
Si	-1.91010400	-1.10279900	1.08731000
Si	-2.14273900	1.23711100	1.28493100
Si	0.00000000	2.47422200	-1.28493100
Si	1.91010400	1.10279900	-1.08731000
Si	2.14273900	-1.23711100	-1.28493100
Si	0.00000000	-2.20559800	-1.08731000
Si	-2.14273900	-1.23711100	-1.28493100
Si	-1.91010400	1.10279900	-1.08731000
Cr	0.00000000	0.00000000	0.00000000

#### **MoSi<sub>12</sub>**

Si	0.00000000	2.36379300	1.20351600
Si	2.04710500	1.18189700	1.20351600
Si	2.04710500	-1.18189700	1.20351600
Si	0.00000000	-2.36379300	1.20351600
Si	-2.04710500	-1.18189700	1.20351600
Si	-2.04710500	1.18189700	1.20351600
Si	0.00000000	2.36379300	-1.20351600
Si	2.04710500	1.18189700	-1.20351600
Si	2.04710500	-1.18189700	-1.20351600
Si	0.00000000	-2.36379300	-1.20351600
Si	-2.04710500	-1.18189700	-1.20351600
Si	-2.04710500	1.18189700	-1.20351600
Mo	0.00000000	0.00000000	0.00000000

#### **WSi<sub>12</sub>**

Si	0.00000000	2.36314600	1.20888100
Si	2.04654400	1.18157300	1.20888100
Si	2.04654400	-1.18157300	1.20888100
Si	0.00000000	-2.36314600	1.20888100
Si	-2.04654400	-1.18157300	1.20888100
Si	-2.04654400	1.18157300	1.20888100
Si	0.00000000	2.36314600	-1.20888100
Si	2.04654400	1.18157300	-1.20888100
Si	2.04654400	-1.18157300	-1.20888100
Si	0.00000000	-2.36314600	-1.20888100
Si	-2.04654400	-1.18157300	-1.20888100

Si	-2.04654400	1.18157300	-1.20888100
W	0.00000000	0.00000000	0.00000000

**W<sub>2</sub>Si<sub>18</sub>**

Si	-2.07978800	-1.20076600	2.37240700
Si	-2.07978800	1.20076600	2.37240700
Si	0.00000000	2.40153300	2.37240700
Si	2.07978800	1.20076600	2.37240700
Si	2.07978800	-1.20076600	2.37240700
Si	0.00000000	-2.40153300	2.37240700
Si	-2.27329000	-1.06617700	0.00000000
Si	-2.05998200	1.43563800	0.00000000
Si	0.21330800	2.50181600	0.00000000
Si	2.27329000	1.06617700	0.00000000
Si	2.05998200	-1.43563800	0.00000000
Si	-0.21330800	-2.50181600	0.00000000
W	0.00000000	0.00000000	1.24701500
Si	-2.07978800	1.20076600	-2.37240700
Si	-2.07978800	-1.20076600	-2.37240700
Si	0.00000000	-2.40153300	-2.37240700
Si	2.07978800	-1.20076600	-2.37240700
Si	2.07978800	1.20076600	-2.37240700
Si	0.00000000	2.40153300	-2.37240700
W	0.00000000	0.00000000	-1.24701500

**W<sub>4</sub>Si<sub>30</sub>**

Si	-2.14130400	-1.23628200	4.87538700
Si	-2.14130400	1.23628200	4.87538700
Si	0.00000000	2.47256400	4.87538700
Si	2.14130400	1.23628200	4.87538700
Si	2.14130400	-1.23628200	4.87538700
Si	0.00000000	-2.47256400	4.87538700
Si	-2.42371600	-0.01014800	2.62980400
Si	-1.22064600	2.09392600	2.62980400
Si	1.20307000	2.10407300	2.62980400
Si	2.42371600	0.01014800	2.62980400
Si	1.22064600	-2.09392600	2.62980400
Si	-1.20307000	-2.10407300	2.62980400
W	0.00000000	0.00000000	3.96925100
Si	-2.50231700	-0.09296400	-0.16321800
Si	-1.33166800	2.12058800	-0.16321800
Si	1.17065000	2.21355200	-0.16321800
Si	2.50231700	0.09296400	-0.16321800
Si	1.33166800	-2.12058800	-0.16321800

Si	-1.17065000	-2.21355200	-0.16321800
W	0.00000000	0.00000000	1.44167900
Si	-2.48018200	0.15284800	-2.60607500
Si	-1.10772100	2.22432400	-2.60607500
Si	1.37246100	2.07147700	-2.60607500
Si	2.48018200	-0.15284800	-2.60607500
Si	1.10772100	-2.22432400	-2.60607500
Si	-1.37246100	-2.07147700	-2.60607500
W	0.00000000	0.00000000	-1.26670100
Si	-2.38464300	-0.05809800	-4.98780000
Si	-1.24263600	2.03611200	-4.98780000
Si	1.14200700	2.09421100	-4.98780000
Si	2.38464300	0.05809800	-4.98780000
Si	1.24263600	-2.03611200	-4.98780000
Si	-1.14200700	-2.09421100	-4.98780000
W	0.00000000	0.00000000	-3.85828500

**W<sub>6</sub>Si<sub>42</sub>**

Si	2.20037800	1.25135400	2.31414900
Si	2.18389300	-1.27990600	2.31414900
Si	-0.01648500	-2.53126000	2.31414900
Si	-2.20037800	-1.25135400	2.31414900
Si	-2.18389300	1.27990600	2.31414900
Si	0.01648500	2.53126000	2.31414900
Si	2.40439400	0.00000000	0.03086300
Si	1.20219700	-2.08226600	0.03086300
Si	-1.20219700	-2.08226600	0.03086300
Si	-2.40439400	0.00000000	0.03086300
Si	-1.20219700	2.08226600	0.03086300
Si	1.20219700	2.08226600	0.03086300
W	0.00000000	0.00000000	1.37704700
Si	2.49550600	0.06642400	-2.75454300
Si	1.30527800	-2.12796000	-2.75454300
Si	-1.19022800	-2.19438400	-2.75454300
Si	-2.49550600	-0.06642400	-2.75454300
Si	-1.30527800	2.12796000	-2.75454300
Si	1.19022800	2.19438400	-2.75454300
W	0.00000000	0.00000000	-1.23330300
Si	2.47746000	-0.19912600	-5.19930800
Si	1.06628200	-2.24510600	-5.19930800
Si	-1.41117800	-2.04598000	-5.19930800
Si	-2.47746000	0.19912600	-5.19930800
Si	-1.06628200	2.24510600	-5.19930800
Si	1.41117800	2.04598000	-5.19930800

W	0.00000000	0.00000000	-3.90205700
Si	2.39322000	0.04442100	-7.58066700
Si	1.23508000	-2.05037900	-7.58066700
Si	-1.15814000	-2.09480000	-7.58066700
Si	-2.39322000	-0.04442100	-7.58066700
Si	-1.23508000	2.05037900	-7.58066700
Si	1.15814000	2.09480000	-7.58066700
W	0.00000000	0.00000000	-6.46075500
Si	2.45683600	-0.02732400	7.52727400
Si	1.20475500	-2.14134400	7.52727400
Si	-1.25208100	-2.11402000	7.52727400
Si	-2.45683600	0.02732400	7.52727400
Si	-1.20475500	2.14134400	7.52727400
Si	1.25208100	2.11402000	7.52727400
Si	2.09037900	-1.23608000	5.28255600
Si	-0.02528700	-2.42836100	5.28255600
Si	-2.11566600	-1.19228100	5.28255600
Si	-2.09037900	1.23608000	5.28255600
Si	0.02528700	2.42836100	5.28255600
Si	2.11566600	1.19228100	5.28255600
W	0.00000000	0.00000000	6.60801600
W	0.00000000	0.00000000	4.04203600

(2)  $\text{WSi}_{12}\text{-N}_2\text{O}$  and  $\text{WSi}_{12}\text{-CO}$  compounds

**$\text{WSi}_{12}\text{-N}_2\text{O}$**

Si	0.38093200	-0.35411100	-2.49244700
Si	2.08810200	-0.84271300	-1.01485700
Si	2.11312200	0.36000900	1.21481000
Si	0.43529800	1.88407000	1.65464500
Si	-1.30636100	2.29037300	0.12052700
Si	-1.33292100	1.17164400	-1.95701700
Si	-0.85918200	-2.23348500	-1.46510400
Si	0.89380200	-2.59743300	0.04454300
Si	0.92135000	-1.47596000	2.12690500
Si	-0.80425200	0.00650600	2.68358500
Si	-2.55459600	0.49018300	1.13900800
Si	-2.58049300	-0.65515700	-0.98477400
W	-0.24068100	-0.18042100	0.09862800
N	2.07137500	3.17361300	-1.08762100
N	2.02271100	2.63825500	-2.04227800
O	3.20307200	0.00664300	-0.04583700
<b>A</b>			
Si	0.95742800	-2.02716000	-1.11303400
Si	2.06080600	0.00005300	-1.29897000

Si	0.95733600	2.02721600	-1.11304500
Si	-1.39399500	2.02973400	-1.29203900
Si	-2.59812800	-0.00006400	-1.44440700
Si	-1.39389900	-2.02980100	-1.29201300
Si	0.70444300	-1.99973100	1.30419700
Si	1.80469400	0.00003100	1.80558900
Si	0.70441200	1.99976400	1.30417600
Si	-1.65411000	2.06890500	1.13265700
Si	-2.80303100	-0.00001500	0.96232800
Si	-1.65408000	-2.06892000	1.13266700
W	-0.35357500	-0.00000100	0.01665800
N	4.19565700	-0.00001600	0.29226900
N	2.87968000	0.00004600	0.33519100
O	4.61887400	-0.00003700	-0.85730100
<b>B</b>			
Si	-0.50865100	2.31711300	1.38951400
Si	1.22924200	0.89061700	2.02773800
Si	0.91458800	-1.44855800	1.93094800
Si	-1.12288400	-2.29462300	1.15082600
Si	-2.82531700	-0.87973000	0.33184000
Si	-2.50101000	1.47148600	0.45488000
Si	0.35955700	2.40811100	-0.89048800
Si	2.10169500	1.09758200	-0.15916800
Si	1.70494800	-1.63780600	-0.28934400
Si	-0.29652100	-2.38753500	-1.15527600
Si	-1.93998900	-0.86586200	-1.91826700
Si	-1.61809500	1.48676200	-1.79540500
W	-0.34383800	0.00457700	0.06657700
N	4.22398700	-0.53932000	-0.98073600
N	2.90344600	-0.40400900	-0.74748600
O	4.82326200	0.50735600	-0.98979100
<b>C</b>			
Si	1.58948700	-1.96407500	-1.18176300
Si	1.58754300	-2.00528600	1.11275100
Si	1.58320200	-0.03871300	2.29575300
Si	1.58100700	1.96927700	1.18447700
Si	1.58275500	2.01038400	-1.11003800
Si	1.58709300	0.04387000	-2.29314400
Si	-0.77613000	-2.16597000	-1.30250700
Si	-0.77817800	-2.21131500	1.22271800
Si	-0.78325300	-0.04691100	2.52474100
Si	-0.78543700	2.16332500	1.30143500
Si	-0.78341900	2.20899700	-1.22444700
Si	-0.77898600	0.04384600	-2.52608600

W	0.06841600	0.00003700	0.00002900
N	-3.23012600	-0.00501300	-0.00268000
N	-2.10228100	-0.00328800	-0.00184700
O	-4.41194300	-0.00608000	-0.00311900

**WSi<sub>12</sub>-CO**

Si	0.56293000	-2.23203800	-1.43334700
Si	2.21506700	-0.62875000	-1.43370200
Si	1.65162700	1.60353500	-1.43371800
Si	-0.56292300	2.23194200	-1.43345400
Si	-2.21505400	0.62869900	-1.43377800
Si	-1.65164700	-1.60359000	-1.43361800
Si	0.61948700	-2.45671900	0.93902900
Si	2.43720800	-0.69143700	0.93891000
Si	1.81758200	1.76490000	0.93869200
Si	-0.61948200	2.45665500	0.93883000
Si	-2.43707000	0.69164600	0.93879300
Si	-1.81777100	-1.76473400	0.93883400
W	0.00002000	-0.00006600	0.05006500
C	-0.00001200	0.00012600	2.04348800
O	-0.00009000	0.00032400	3.19920900

**a**

Si	-2.47749600	-1.18095100	0.44285300
Si	-2.47736300	1.18120000	0.44280800
Si	-0.63752500	2.28843500	1.34909000
Si	1.31739400	1.17424700	1.95445600
Si	1.31733800	-1.17437600	1.95438500
Si	-0.63776800	-2.28832100	1.34916600
Si	-1.63983700	-1.21649600	-1.83543500
Si	-1.63960500	1.21678300	-1.83545400
Si	0.11511600	2.53092300	-0.92440900
Si	2.05564800	1.48007000	-0.26208100
Si	2.05537300	-1.48039300	-0.26221700
Si	0.11462800	-2.53097400	-0.92440200
W	-0.15241300	0.00001100	0.05223600
C	2.96468200	-0.00021800	-1.15172000
O	3.62098500	-0.00020300	-2.15472000

**b**

Si	-1.45755400	2.02901800	-1.04848700
Si	-2.70308900	-0.00000500	-1.09136400
Si	-1.45754400	-2.02902200	-1.04848700
Si	0.90841900	-2.08962400	-1.38432000
Si	1.89244500	0.00000700	-1.54565700
Si	0.90840900	2.08963200	-1.38431500

Si	-1.30390300	2.06577000	1.37512100
Si	-2.42440900	-0.00000700	1.29374600
Si	-1.30389200	-2.06577900	1.37512200
Si	1.02205300	-1.94720900	1.05119200
Si	2.10959600	0.00000500	1.82729400
Si	1.02204300	1.94721400	1.05119700
W	-0.20553000	0.00000000	-0.09292800
C	3.20091700	0.00000900	0.07238900
O	4.37846400	-0.00000600	-0.01902800

(3) Transition states involved in the CO oxidation reaction

1) CrSi<sub>12</sub>

**TS1**

Si	-0.52929900	2.32904600	-1.32210000
Si	-1.95859100	1.22032700	0.12935900
Si	-1.79157500	-1.47136700	0.17588100
Si	0.20666800	-2.49001200	-0.34256100
Si	1.69397000	-1.46317000	-1.86126800
Si	1.24231900	0.89436400	-1.97502700
Si	0.76545400	2.38016400	0.68294300
Si	-0.90530800	1.62832800	2.16947200
Si	-0.73993200	-0.73745200	2.22427000
Si	1.18379400	-2.07456300	1.79092800
Si	2.53179000	-0.86645200	0.25349200
Si	2.71926600	1.45302300	-0.14933300
O	-3.24992500	0.23292500	-0.04633200
C	-2.73215200	-1.03734000	-1.39637300
O	-3.26479300	-1.00188500	-2.40876500
Cr	0.27712000	0.04768400	0.13142600

**TS2**

Si	-0.85033800	-2.14599500	1.17690800
Si	-2.91784300	-1.32526100	0.33596800
Si	-2.66358100	1.00865400	0.11616500
Si	-1.17659500	2.50387200	1.20007200
Si	0.66789700	1.22334400	1.93668100
Si	0.99112300	-1.11218300	2.23599800
Si	0.16607900	-2.54801900	-0.94241100
Si	-1.63458100	-1.19253200	-1.67939500
Si	-1.80000800	1.13951000	-2.10082100
Si	-0.07109500	2.26226900	-0.91588900
Si	1.86980300	1.31090300	-0.07129900
Si	1.72262700	-1.09191300	-0.02406200
C	3.94084600	0.09261000	-0.84087200
O	4.80447800	0.87091400	-0.94203200

O	3.57125400	-1.07138400	-0.96896800
Cr	-0.45415800	0.02462600	0.10760100

## 2) MoSi<sub>12</sub>

### TS1

Si	-0.26138100	2.28479900	-1.29927300
Si	-1.93780100	1.45834200	0.06729600
Si	-1.96934100	-1.26723100	0.17265700
Si	-0.13661500	-2.58144100	-0.40099700
Si	1.49867200	-1.55416800	-1.77071900
Si	1.40280500	0.80483800	-2.13764100
Si	1.01819000	2.45372500	0.73769500
Si	-0.75190200	1.64986000	2.06987400
Si	-0.89313400	-0.71761500	2.32157600
Si	0.92164900	-2.11301800	1.69159100
Si	2.60548700	-1.15447200	0.29488500
Si	2.74110800	1.15923900	-0.15582000
O	-3.28410700	0.53495700	-0.04724000
C	-2.94180100	-0.83881800	-1.38266200
O	-3.50935000	-0.78606300	-2.37317800
Mo	0.30167000	0.02670800	0.12818100

### TS2

Si	-1.00818400	-2.23234900	1.27742300
Si	-2.84691500	-1.15999200	0.20794600
Si	-2.73695800	1.19570000	0.02861600
Si	-1.02349900	2.47081300	1.05819100
Si	0.74134100	1.27563400	2.10364800
Si	0.84055400	-1.09906500	2.23754500
Si	0.04997000	-2.49977200	-0.86304100
Si	-1.64522900	-1.18307000	-1.86732000
Si	-1.53100800	1.17856900	-2.06036400
Si	0.23829800	2.33301800	-0.97618800
Si	1.97541600	1.16810000	0.08282800
Si	1.80478100	-1.27369500	0.02335900
C	3.92445200	-0.02274200	-0.90300500
O	4.87241400	0.65689100	-0.85061900
O	3.42501500	-1.07955500	-1.28594100
Mo	-0.42728800	0.02579200	0.11841700

## 3) WSi<sub>12</sub>

### TS1

Si	-0.29494700	2.28126100	-1.30512100
Si	-1.96530900	1.47392600	0.07241100
Si	-2.00983300	-1.24399000	0.17322100



Si	-0.20967800	-2.59416400	-0.42095800
Si	1.41995600	-1.55979600	-1.79319900
Si	1.34703200	0.79364300	-2.18025100
Si	1.01239700	2.45674800	0.72528100
Si	-0.74386500	1.63459200	2.06066000
Si	-0.90866300	-0.72752600	2.32612400
Si	0.88929900	-2.11516800	1.65507100
Si	2.58305700	-1.17868100	0.25884500
Si	2.70108500	1.13631800	-0.19262900
W	0.26865700	0.02086600	0.10658100
O	-3.31524600	0.54818600	-0.02683600
C	-3.01076300	-0.81385500	-1.36833900
O	-3.59769300	-0.75584600	-2.34683100

### TS2

Si	-1.03320200	-2.23318300	1.26493800
Si	-2.80182900	-1.10769900	0.14285100
Si	-2.67053500	1.24625700	-0.02212300
Si	-0.93537800	2.46683500	1.02529900
Si	0.77923800	1.26121400	2.13628400
Si	0.80645500	-1.11141000	2.24450100
Si	0.06962500	-2.49546000	-0.86815300
Si	-1.57429000	-1.16108600	-1.92455600
Si	-1.39509600	1.19669800	-2.08116000
Si	0.37689500	2.32900300	-0.98318200
Si	2.04403700	1.11661900	0.12889900
Si	1.85179800	-1.33323700	0.04400100
W	-0.36637700	0.02232600	0.10196900
C	3.92189000	-0.04900900	-0.91218700
O	4.89537700	0.59546000	-0.84012400
O	3.39619000	-1.07068300	-1.35725000

### 4) W<sub>2</sub>Si<sub>18</sub>

#### TS1

Si	2.52633200	-0.48891900	-2.48929200
Si	2.01921900	-2.47144500	-1.23220800
Si	2.14635000	-2.54970500	1.17154600
Si	2.55166100	-0.54298300	2.36332600
Si	3.11974200	1.47053400	1.10486500
Si	2.96009800	1.55452300	-1.33501200
Si	0.16725300	-0.21420100	-2.46231700
Si	-0.48369300	-2.16828000	-1.31429900
Si	-0.19174800	-2.20488200	1.04253900
Si	0.29693600	0.20136100	2.46175000
Si	0.84711800	2.23176400	1.38495700

Si	0.70451700	2.19585800	-1.04357000
W	1.47487700	-0.21849800	-0.02233900
Si	-2.73153700	-1.08641000	-1.21820400
Si	-1.95668800	0.79799600	-2.48773400
Si	-1.57509000	2.73249800	-1.21556300
Si	-1.59297600	2.51457700	1.21896000
Si	-2.04060900	0.55277100	2.63357100
Si	-2.33003900	-1.39075200	1.42518600
W	-0.97073000	0.34326000	0.01598900
O	-3.56348400	-2.10287100	0.60899600
C	-4.43858900	-0.72923500	-0.46969800
O	-5.53540900	-0.48928000	-0.21286400

**TS2**

Si	-2.43722200	-1.14077300	2.34512700
Si	-1.82668100	-2.84669400	0.80944800
Si	-1.88138000	-2.43727900	-1.56429600
Si	-2.55873200	-0.31177600	-2.43294700
Si	-3.23573500	1.43769300	-0.96407000
Si	-3.16778200	0.98398300	1.41893200
Si	-0.32763000	-0.07232900	2.48994000
Si	0.45591400	-2.19510200	0.80396400
Si	0.50190200	-1.92046300	-1.55617400
Si	-0.23849900	0.22034300	-2.46477100
Si	-0.98941500	2.21673700	-0.96797900
Si	-0.99931600	2.02085200	1.52040400
W	-1.46245500	-0.35011800	-0.02160400
Si	2.62432900	-1.29095000	0.97328200
Si	1.98667900	0.34896000	2.52698600
Si	1.35732600	2.49760600	1.62109200
Si	1.23817900	2.98704000	-0.74822400
Si	1.84109600	1.35155900	-2.35700700
Si	2.67409900	-0.68425900	-1.46568900
W	0.89690000	0.46105200	0.05235000
O	4.65753900	-0.28390100	-0.80804400
C	4.86313300	-1.18124600	0.01797700
O	5.64651800	-1.89531500	0.53112700

5)  $W_4Si_{30}$

**TS1**

Si	5.10928700	-1.27586900	-2.16471800
Si	4.92752700	-2.64849100	-0.10432300
Si	4.95239100	-1.50981900	2.09426900
Si	5.10458500	0.94674200	2.21845300
Si	5.21582200	2.29839300	0.15807000

Si	5.22679600	1.17974000	-2.02390900
Si	2.76516600	-2.06056300	-1.38149500
Si	2.69388800	-2.20079000	1.05403300
Si	2.78885500	-0.16107200	2.39598000
Si	2.93256600	1.99229100	1.26372800
Si	2.96265300	2.09662500	-1.17269500
Si	2.90872400	0.07424100	-2.48639200
W	4.17556300	-0.12008800	-0.00034500
Si	-0.07548700	-2.02524900	-1.25918200
Si	-0.05116900	-2.16940800	1.22445700
Si	0.07485600	-0.10602500	2.50586800
Si	0.23454300	2.14789700	1.27676600
Si	0.05803100	2.28318900	-1.27774800
Si	0.00442900	0.15882200	-2.53502100
W	1.65287200	0.01657300	-0.06253300
Si	-2.69616200	-2.09982100	-1.31493900
Si	-2.48899100	-2.10673400	1.10125600
Si	-2.37772000	0.02690000	2.47654800
Si	-2.25654500	2.24249900	1.55930100
Si	-2.28066400	2.41463200	-0.81409700
Si	-2.36598200	-0.04682700	-2.37676200
W	-1.04146700	0.11763800	0.02472000
Si	-5.09615100	-1.43381400	-1.35130600
Si	-4.78296700	-1.78163200	1.28928300
Si	-4.78916000	0.17941900	2.51030200
Si	-4.70091100	2.22041000	1.25727100
Si	-4.60428300	2.49470600	-1.13720300
Si	-4.61397800	0.59391100	-2.50618500
W	-3.63759100	0.21802100	0.01544200
O	-5.83558400	-2.65819400	0.38478400
C	-6.87137700	-1.44932700	-0.69032800
O	-8.00752400	-1.41967100	-0.49622600

**TS2**

Si	5.00889200	1.62978400	2.01455100
Si	4.93922500	2.68297700	-0.22445000
Si	5.01689600	1.27425700	-2.25331600
Si	5.16077200	-1.18099900	-2.05151000
Si	5.23632700	-2.23482900	0.18111600
Si	5.15983800	-0.82833800	2.21486600
Si	2.71393900	2.28570200	1.01420100
Si	2.72112600	2.06929200	-1.39965800
Si	2.84203400	-0.12344400	-2.42118300
Si	2.97138000	-2.11073100	-1.03409100
Si	2.97088400	-1.88244900	1.38177500

Si	2.83653900	0.30883200	2.41238100
W	4.18108400	0.17027800	-0.01302000
Si	-0.09139600	2.20193200	1.04399500
Si	-0.07284100	1.90208500	-1.45367200
Si	0.05091600	-0.36659000	-2.48489800
Si	0.19310200	-2.38004500	-1.04262000
Si	0.21596000	-2.06284700	1.47879100
Si	0.02096300	0.22021000	2.53053300
W	1.65739300	0.01779600	-0.00249200
Si	-2.51732300	1.95294100	1.14854900
Si	-2.57171400	1.95863400	-1.29657100
Si	-2.38496200	-0.18083700	-2.42236900
Si	-2.24465700	-2.41065300	-1.12053100
Si	-2.24070900	-2.38030400	1.33378800
Si	-2.37437000	-0.22430900	2.49202800
W	-1.03917300	-0.15806400	0.02638600
Si	-4.86987100	1.76423300	0.98196300
Si	-4.95836700	1.36232300	-1.47795600
Si	-4.68890400	-0.77165000	-2.43321500
Si	-4.60578200	-2.59258600	-0.91183400
Si	-4.64700600	-2.25453400	1.46406800
Si	-4.73998700	-0.08115500	2.44554300
W	-3.62608200	-0.31745700	0.02091900
O	-7.00596400	1.69151800	-0.98065100
C	-6.94768800	2.50525000	-0.05196700
O	-7.47466100	3.38135300	0.53255300

6)  $W_6Si_{42}$

**TS1**

Si	-2.52606200	0.98294000	-2.33901900
Si	-2.42730400	2.48000200	-0.27135200
Si	-2.42714200	1.42150400	2.03726200
Si	-2.60290200	-1.08232300	2.23906200
Si	-2.60817900	-2.55792000	0.20446700
Si	-2.56798600	-1.52909700	-2.07298300
Si	-0.21693500	1.84800900	-1.46635800
Si	-0.16329200	2.06347000	0.93964400
Si	-0.22066700	0.07992900	2.35202200
Si	-0.29411600	-2.08746300	1.32812500
Si	-0.26781200	-2.28583000	-1.07815200
Si	-0.26502000	-0.32960000	-2.47625800
W	-1.57851800	-0.07186600	-0.04314000
Si	2.61359300	1.93640600	-1.33079300
Si	2.58187000	2.17616900	1.12427800

Si	2.50284900	0.16055300	2.46671400
Si	2.42800400	-2.13556300	1.35453600
Si	2.62566700	-2.34821900	-1.20118000
Si	2.61320100	-0.27772200	-2.53376100
W	1.03373700	-0.14331800	-0.07849000
Si	5.22460300	2.09683500	-1.39366100
Si	5.02796900	2.21538700	1.01920100
Si	4.95895900	0.15448100	2.48353300
Si	4.90335100	-2.10775500	1.67257200
Si	4.95893400	-2.38674700	-0.69840100
Si	4.98351600	-0.00892300	-2.37197800
W	3.69455700	-0.10880500	0.02642200
Si	7.66509500	1.51152800	-1.39530800
Si	7.33186100	1.96244900	1.24372500
Si	7.37905200	0.04594200	2.54557700
Si	7.35229600	-2.05888700	1.38179800
Si	7.28628100	-2.43442400	-1.00908000
Si	7.25692400	-0.58942600	-2.45639700
W	6.26353200	-0.12880100	0.04537800
O	8.36360200	2.82340300	0.30109000
C	9.43118700	1.60027900	-0.71439800
O	10.56689300	1.60784600	-0.51431000
Si	-7.81944100	-2.08648100	-0.95522800
Si	-7.79621100	-0.09156300	-2.38421800
Si	-7.70008200	2.14843500	-1.37480400
Si	-7.63082200	2.39198100	1.06794300
Si	-7.66985700	0.39698100	2.49769900
Si	-7.75975700	-1.84581000	1.49010900
Si	-5.57104500	-1.33046900	-1.97328000
Si	-5.50643100	1.08019300	-2.21229800
Si	-5.40914900	2.49409800	-0.24513900
Si	-5.39540600	1.50610200	1.97122100
Si	-5.47868100	-0.91069800	2.21770600
Si	-5.55860500	-2.33268800	0.23941400
W	-6.81042400	0.12384700	0.03569600
W	-4.24324600	0.03498800	-0.02539700
<b>TS2</b>			
Si	2.47614400	1.42514500	2.08423600
Si	2.46154400	2.51543100	-0.20685700
Si	2.49154900	1.08369900	-2.28976100
Si	2.55372400	-1.43126000	-2.09179900
Si	2.59786900	-2.52308700	0.18335900
Si	2.55582100	-1.09496000	2.27534500
Si	0.18259800	2.11371200	1.02427500

Si	0.18813900	1.91102700	-1.37108800
Si	0.23275700	-0.26397700	-2.39557500
Si	0.29178000	-2.24920600	-1.02965400
Si	0.29850400	-2.03422800	1.36650800
Si	0.22975100	0.13609600	2.40116000
W	1.58236800	-0.02834200	-0.00289900
Si	-2.61073000	2.14485400	1.05937400
Si	-2.59501600	1.86553000	-1.42896100
Si	-2.55862000	-0.38685600	-2.47926000
Si	-2.49327700	-2.41042700	-1.05247900
Si	-2.46850000	-2.12240400	1.46304700
Si	-2.57639700	0.15277800	2.52265300
W	-1.02669500	-0.09872400	0.00073900
Si	-5.05157900	1.99802000	1.16478100
Si	-5.09524200	2.03094400	-1.27900600
Si	-4.98996000	-0.10118000	-2.42633800
Si	-4.93090000	-2.34442600	-1.15029400
Si	-4.93261500	-2.34519800	1.30942200
Si	-4.98964600	-0.19655700	2.48615000
W	-3.69016800	-0.16026800	0.02492800
Si	-7.41119300	1.90010900	0.98821600
Si	-7.51014700	1.51731500	-1.48592700
Si	-7.31292600	-0.62819800	-2.44727200
Si	-7.29794800	-2.46635800	-0.93578100
Si	-7.33232100	-2.13340700	1.44951000
Si	-7.34977800	0.04218400	2.44689600
W	-6.25199900	-0.22295300	0.01505400
O	-9.54330400	1.90476600	-0.98057400
C	-9.46749300	2.70533200	-0.04206900
O	-9.97327000	3.58573200	0.55413200
Si	7.78693700	-1.88334900	1.37958800
Si	7.72659900	0.32936400	2.44584900
Si	7.66939100	2.35832500	1.06353400
Si	7.67343700	2.18030300	-1.38719500
Si	7.73702300	-0.03274600	-2.45358900
Si	7.79512000	-2.06306800	-1.07166900
Si	5.51713200	-0.96583200	2.18439800
Si	5.44861700	1.45467800	2.00248200
Si	5.41922600	2.50455200	-0.18640900
Si	5.45784800	1.13503700	-2.19305400
Si	5.52666100	-1.28516400	-2.01096100
Si	5.55673300	-2.33583600	0.17705800
W	6.81241600	0.12201800	-0.00422200
W	4.24683500	0.04806100	-0.00393600

7) Two adsorbed N<sub>2</sub>O molecules on WSi<sub>12</sub>

**TS1**

Si	1.38606400	0.99045400	-2.18827000
Si	-0.17567800	2.31501200	-1.05019200
Si	-2.00253500	1.19233400	0.24614500
Si	-1.85093700	-1.41363200	0.09010100
Si	-0.06601100	-2.67519100	-0.71525900
Si	1.53078400	-1.36503200	-1.85364300
Si	2.66337200	1.23281300	-0.10780400
Si	1.00970800	2.44113800	0.99738900
Si	-0.68946800	1.27393800	2.19405600
Si	-0.77011200	-1.11330000	2.31106600
Si	1.06886900	-2.24135100	1.32588100
Si	2.79207500	-1.09759300	0.14701100
W	0.31951500	-0.01742800	0.12732800
O	-1.87296700	2.45593100	-0.83554300
O	-3.33952700	0.28992800	0.22497300
C	-3.16387600	-1.02823500	-1.24375600
O	-3.93834400	-1.00775300	-2.07823900

**TS2**

Si	1.80283500	1.39200000	-1.70574100
Si	-0.08868200	2.40788500	-0.80367500
Si	-2.03477300	0.89573700	-0.12181000
Si	-1.78813400	-1.44804600	-0.33544900
Si	0.19545400	-2.37750000	-1.22012900
Si	1.97978500	-0.97400300	-1.95039200
Si	2.66732900	1.39785000	0.60681000
Si	0.60377800	2.21608400	1.44999000
Si	-1.19843900	0.79236600	2.06891800
Si	-0.81712700	-1.53434700	1.87724400
Si	1.19674900	-2.43671400	0.97913300
Si	2.93324200	-0.95275600	0.27876500
W	0.47560000	-0.06259900	0.08818900
O	-1.80452800	2.30567300	-1.00012000
O	-3.97184600	0.85499100	-0.59454800
C	-4.23670900	-0.34687900	-0.62252400
O	-4.98642500	-1.23393900	-0.72059600

**TS3**

Si	-0.29494700	2.28126100	-1.30512100
Si	-1.96530900	1.47392600	0.07241100
Si	-2.00983300	-1.24399000	0.17322100
Si	-0.20967800	-2.59416400	-0.42095800
Si	1.41995600	-1.55979600	-1.79319900
Si	1.34703200	0.79364300	-2.18025100

Si	1.01239700	2.45674800	0.72528100
Si	-0.74386500	1.63459200	2.06066000
Si	-0.90866300	-0.72752600	2.32612400
Si	0.88929900	-2.11516800	1.65507100
Si	2.58305700	-1.17868100	0.25884500
Si	2.70108500	1.13631800	-0.19262900
W	0.26865700	0.02086600	0.10658100
O	-3.31524600	0.54818600	-0.02683600
C	-3.01076300	-0.81385500	-1.36833900
O	-3.59769300	-0.75584600	-2.34683100
<b>TS4</b>			
Si	-1.03320200	-2.23318300	1.26493800
Si	-2.80182900	-1.10769900	0.14285100
Si	-2.67053500	1.24625700	-0.02212300
Si	-0.93537800	2.46683500	1.02529900
Si	0.77923800	1.26121400	2.13628400
Si	0.80645500	-1.11141000	2.24450100
Si	0.06962500	-2.49546000	-0.86815300
Si	-1.57429000	-1.16108600	-1.92455600
Si	-1.39509600	1.19669800	-2.08116000
Si	0.37689500	2.32900300	-0.98318200
Si	2.04403700	1.11661900	0.12889900
Si	1.85179800	-1.33323700	0.04400100
W	-0.36637700	0.02232600	0.10196900
C	3.92189000	-0.04900900	-0.91218700
O	4.89537700	0.59546000	-0.84012400
O	3.39619000	-1.07068300	-1.35725000