Supplementary Information

Mechanism of Selective and Complete Oxidation in La_2O_3-catalyzed Oxidative Coupling of Methane Reaction

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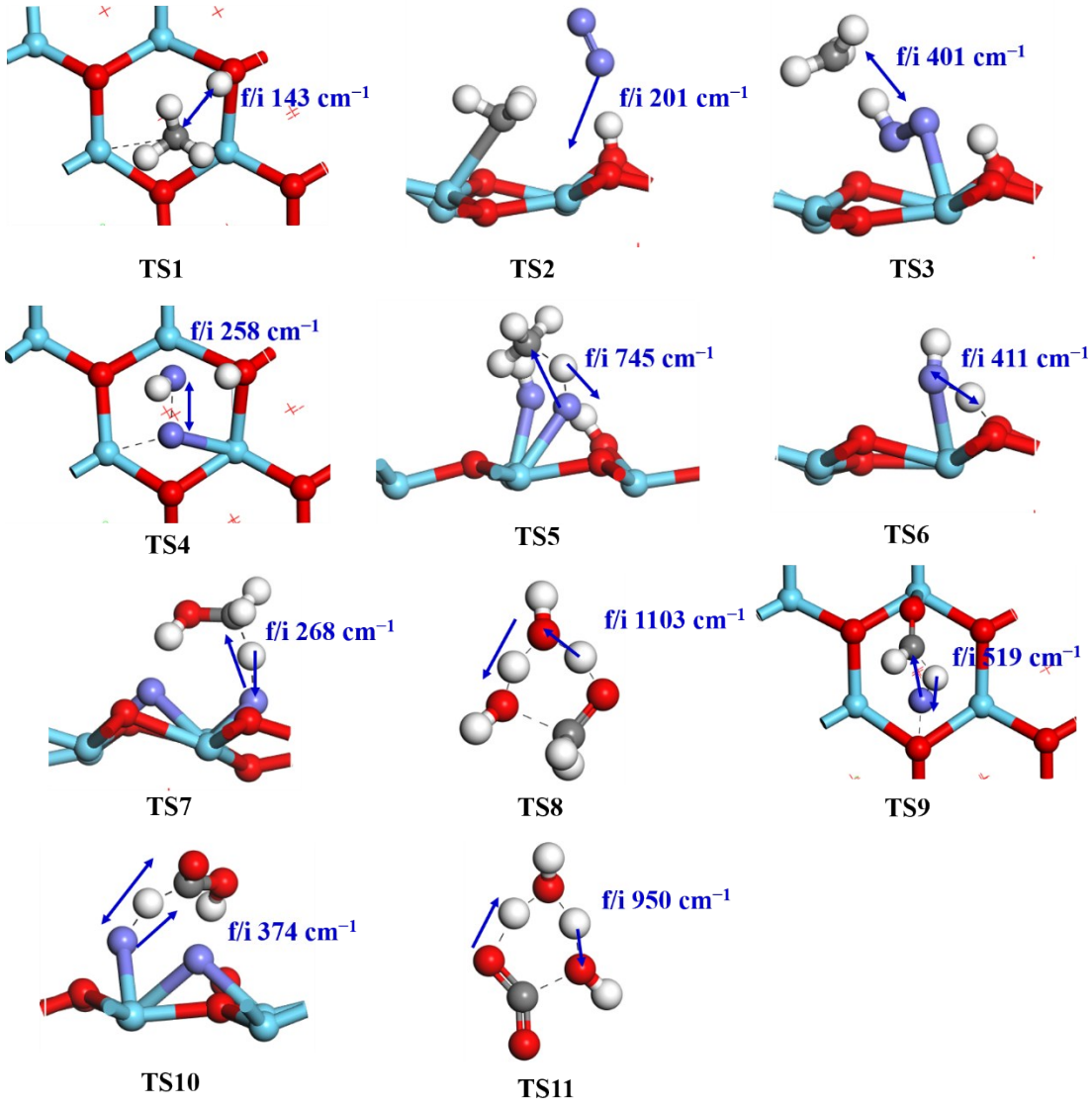

Figrure S2. (a) Spatial distribution of electron localization function (ELF) for CH_4 chemisorption on the bridge La site. Two-dimensional map in the plane of C atom; **(b)** The crystal orbital Hamilton population (COHP) analysis of CH_3–La interaction in CH_4 chemisorption structure.

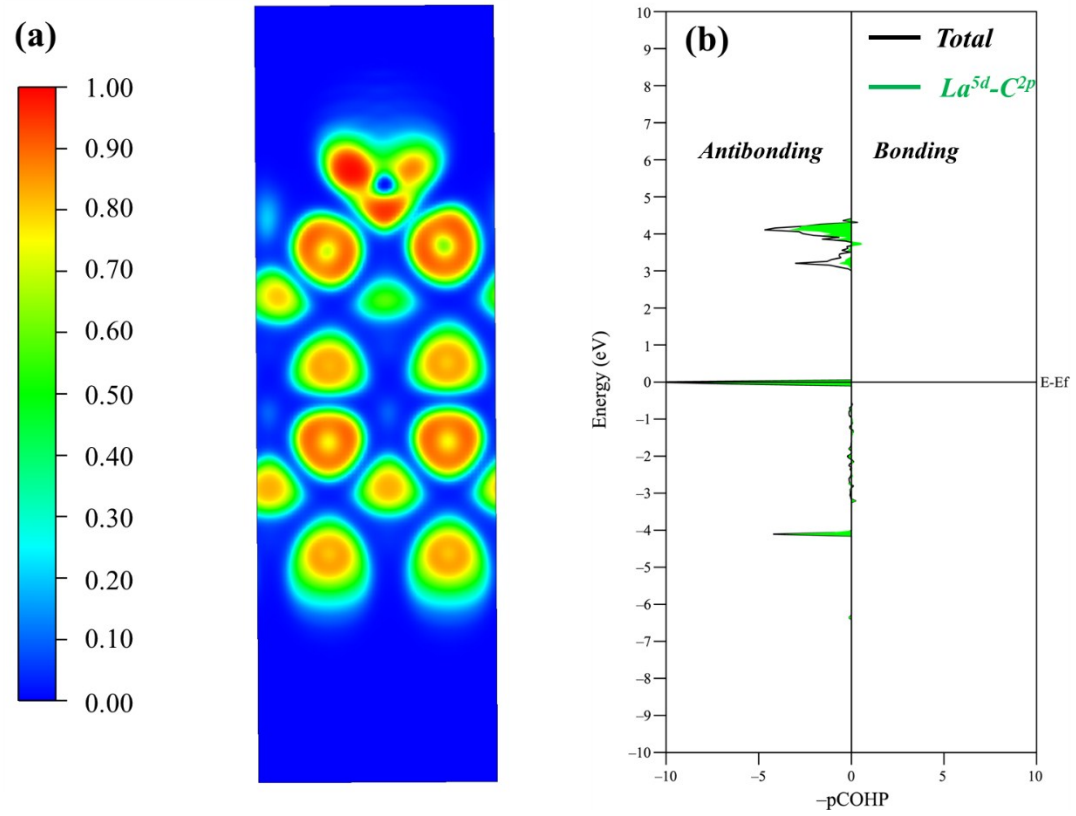

Figure S3. Projected density of states (PDOS) of CH_4 chemisorption on the La_2O_3 (001) surface.

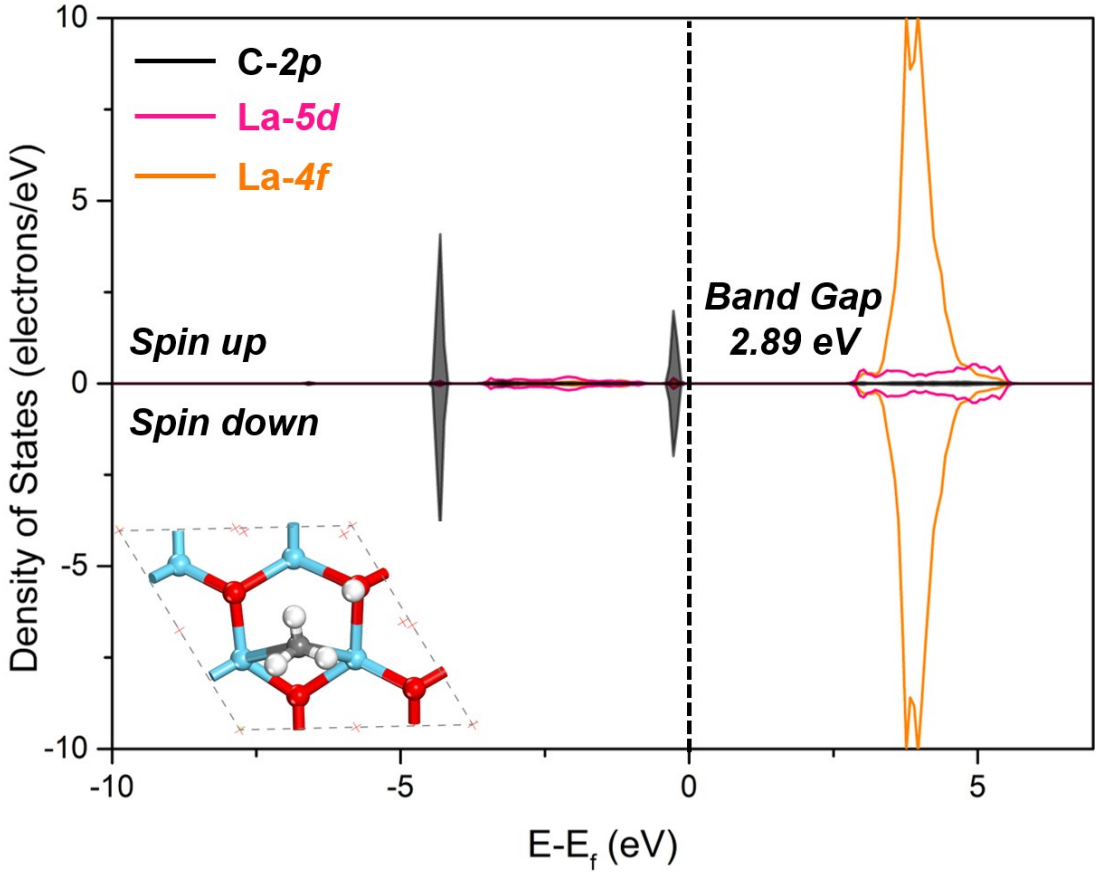

Figure S4. Potential energy surface (ΔE_{0K}, kJ/mol) for CH_4 activation at the O_2^{2-} site on clean and H/OH adsorbed La_2O_3(001) surface

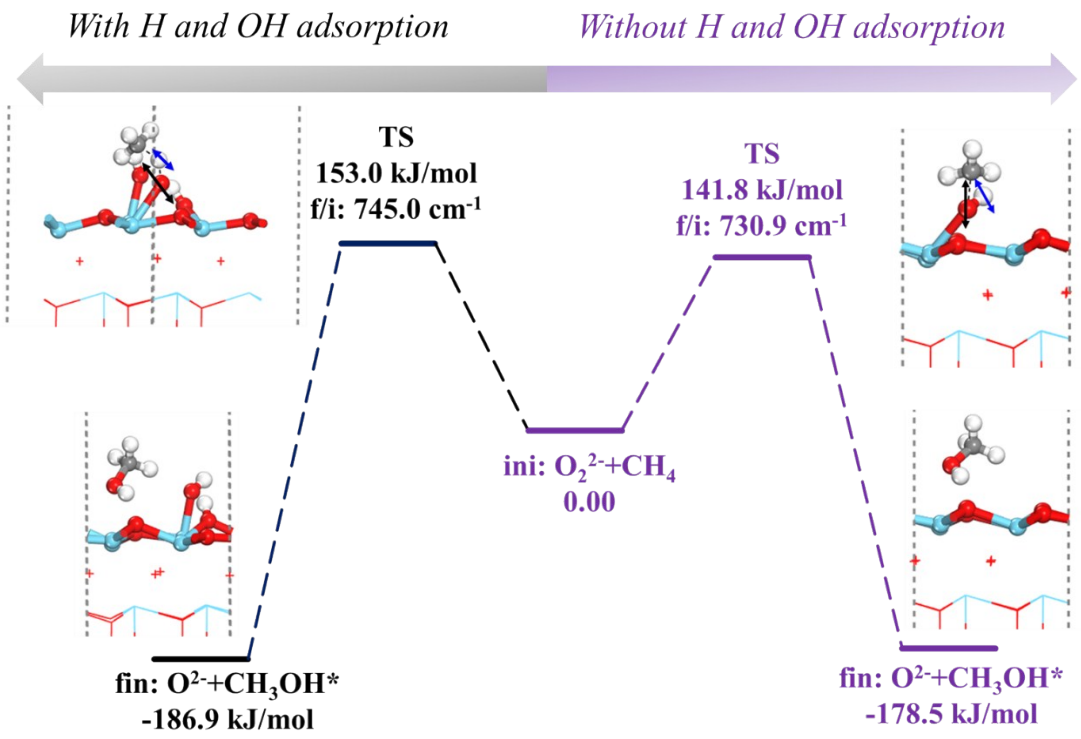

Figure S5. Time evolution of energy in the time scale of 1-800 fs for CH_4 activation at the O_2^{2-} of the clean La_2O_3(001) surface.

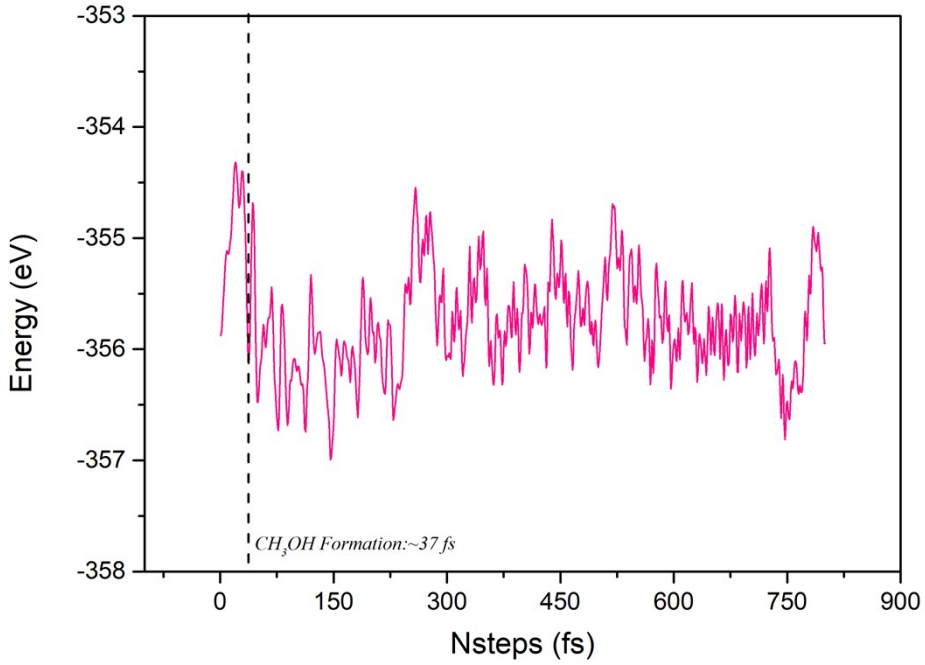

Figure S6. Potential energy surface (ΔG_{823K}, kJ/mol) for CH_4 dissociation at the O^{2-} site on the H-adsorbed $La_2O_3(001)$ surface.

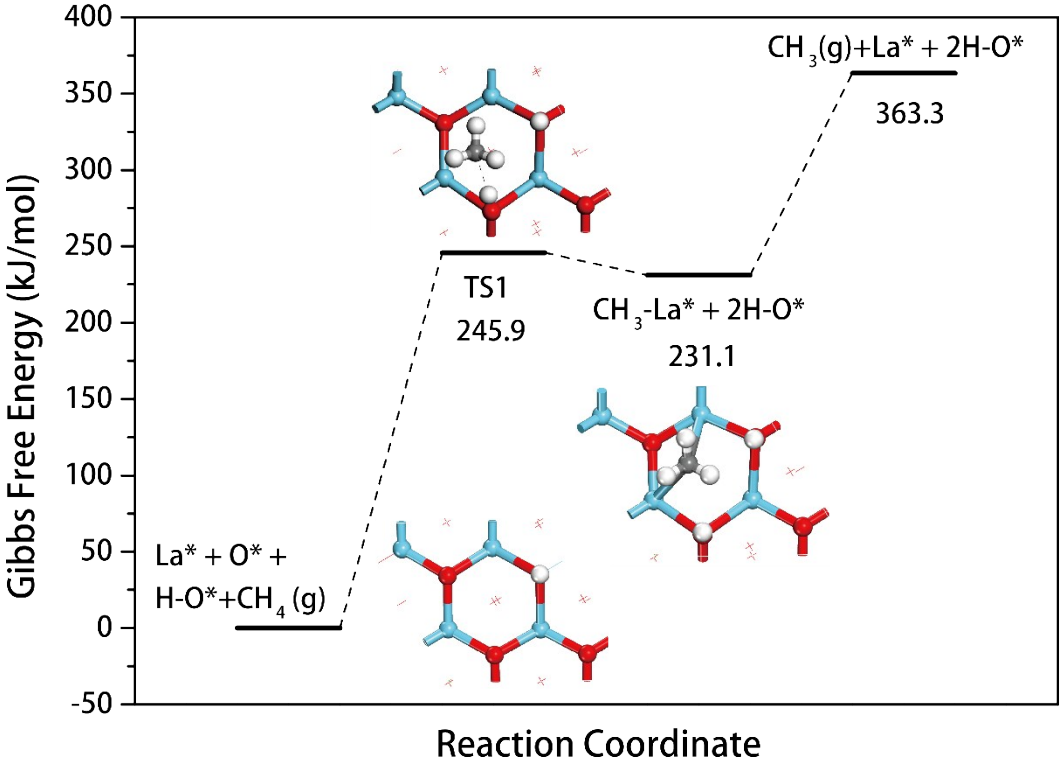

Figure S7. Potential energy surface (ΔE_{0K}, kJ/mol) for CH_3* migration to the lattice oxygen site to form CH_3O* on the La_2O_3(001) surface.

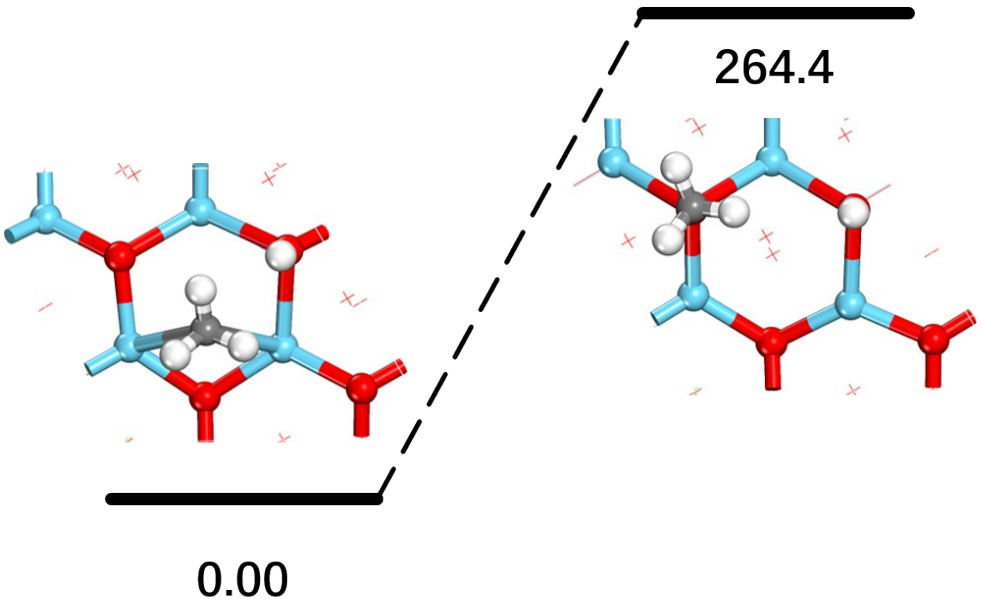

Figure S8. Potential energy surface (ΔG_{823K}, kJ/mol) for CH_3OH dissociation on the $La_2O_3(001)$ surface.

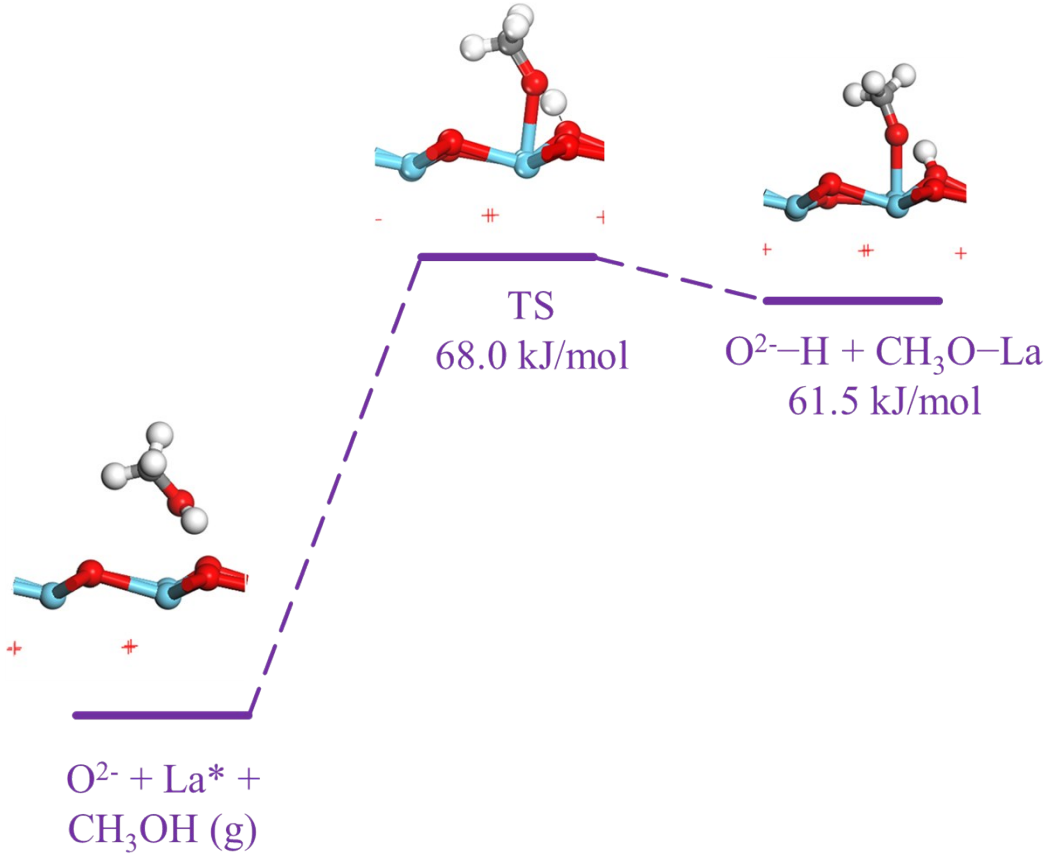

Figure S9. Potential energy surface (ΔG_{823K}, kJ/mol) for CH_3OH dehydrogenation on La_2O_3 (001) surface with two O_2^{2-} sites.

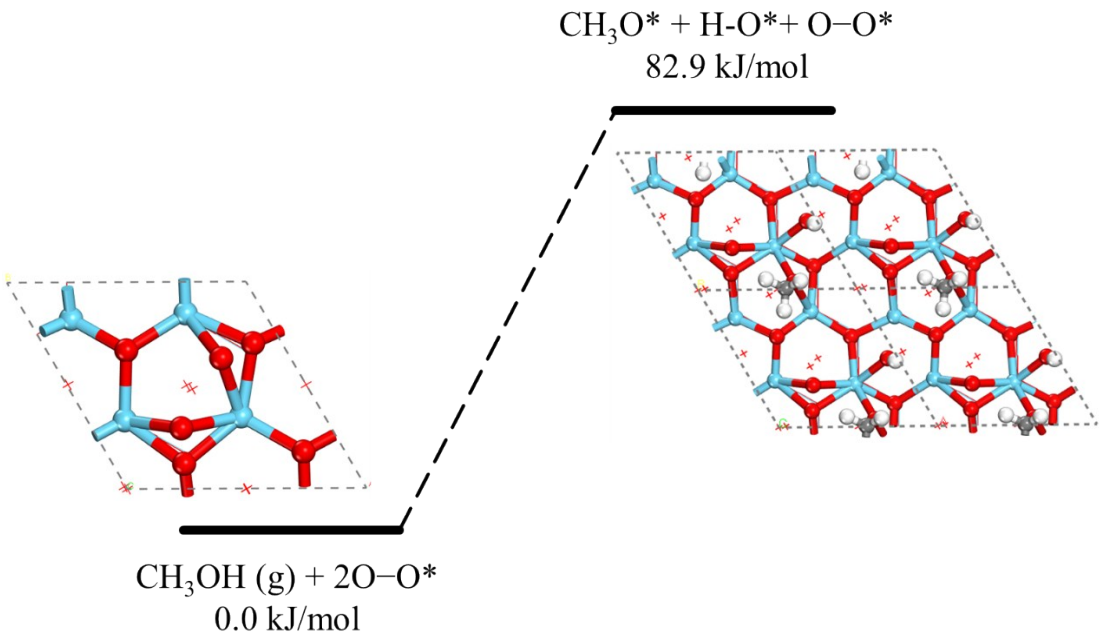

Figure S10. Potential energy surface (ΔG_{823K}, kJ/mol) for CH_2O dehydrogenation on the surface O_2^{2-} site.

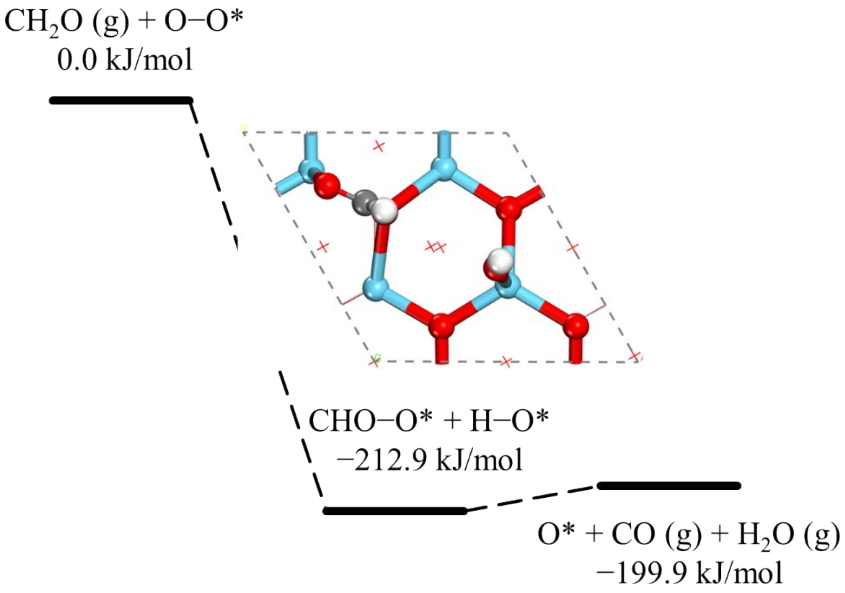

Figure S11. Potential energy surface (ΔG_{823K}, kJ/mol) for gaseous HCOOH dehydration to CO and H_2O.

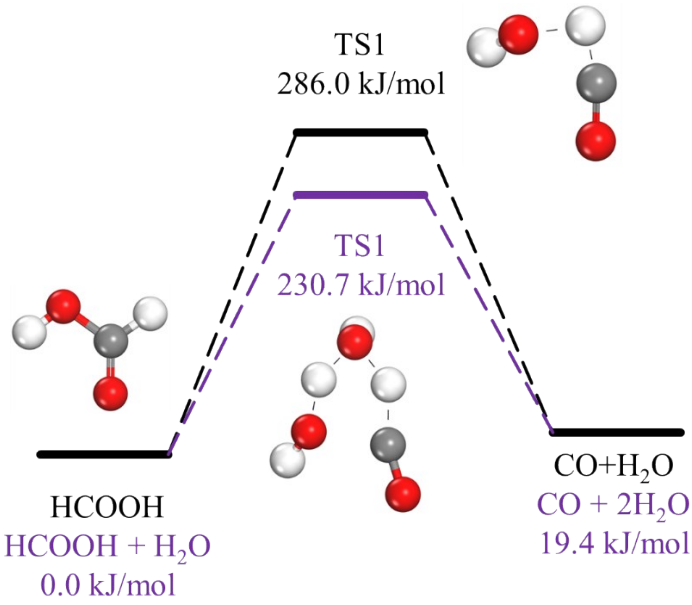

Figure S12. Potential energy surface (ΔE_{0K}, kJ/mol) for CH_4 dissociation at the O^{2-} site on the La_2O_3 (001) surface. (a) CH_3 direct desorption. (b) O_2−assisted CH_3 desorption.

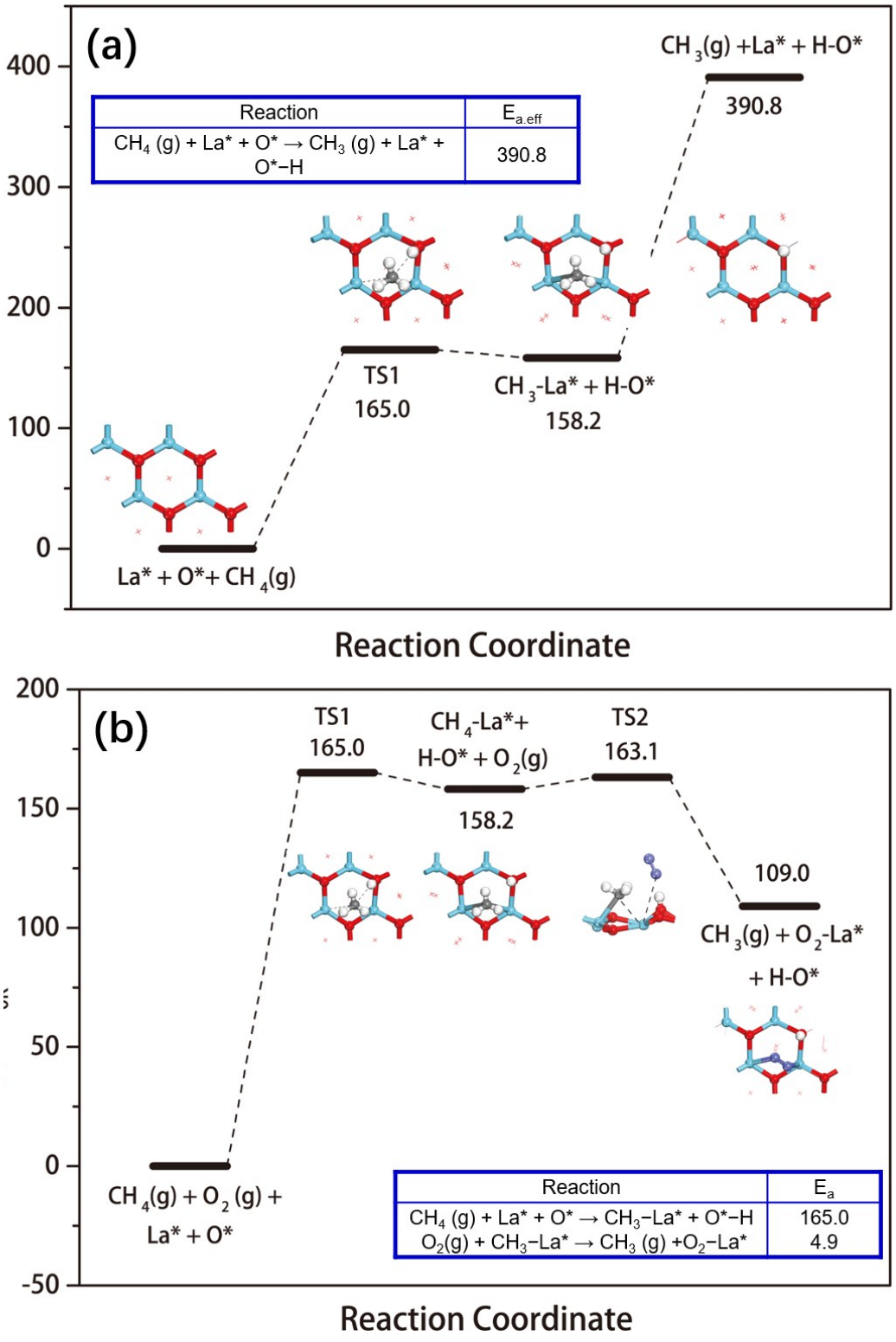

Figure S13. Potential energy surface (ΔE_{0K}, kJ/mol) for CH_4 activation by the $O_2^{\bullet-}$ species and at the O_2^{2-} site on the $La_2O_3(001)$ surface, which continues from that on Figure S9. (a) CH_3 direct formation by reacting with the $O_2^{\bullet-}$ species. (b) CH_3OH direct formation at the O_2^{2-} site.

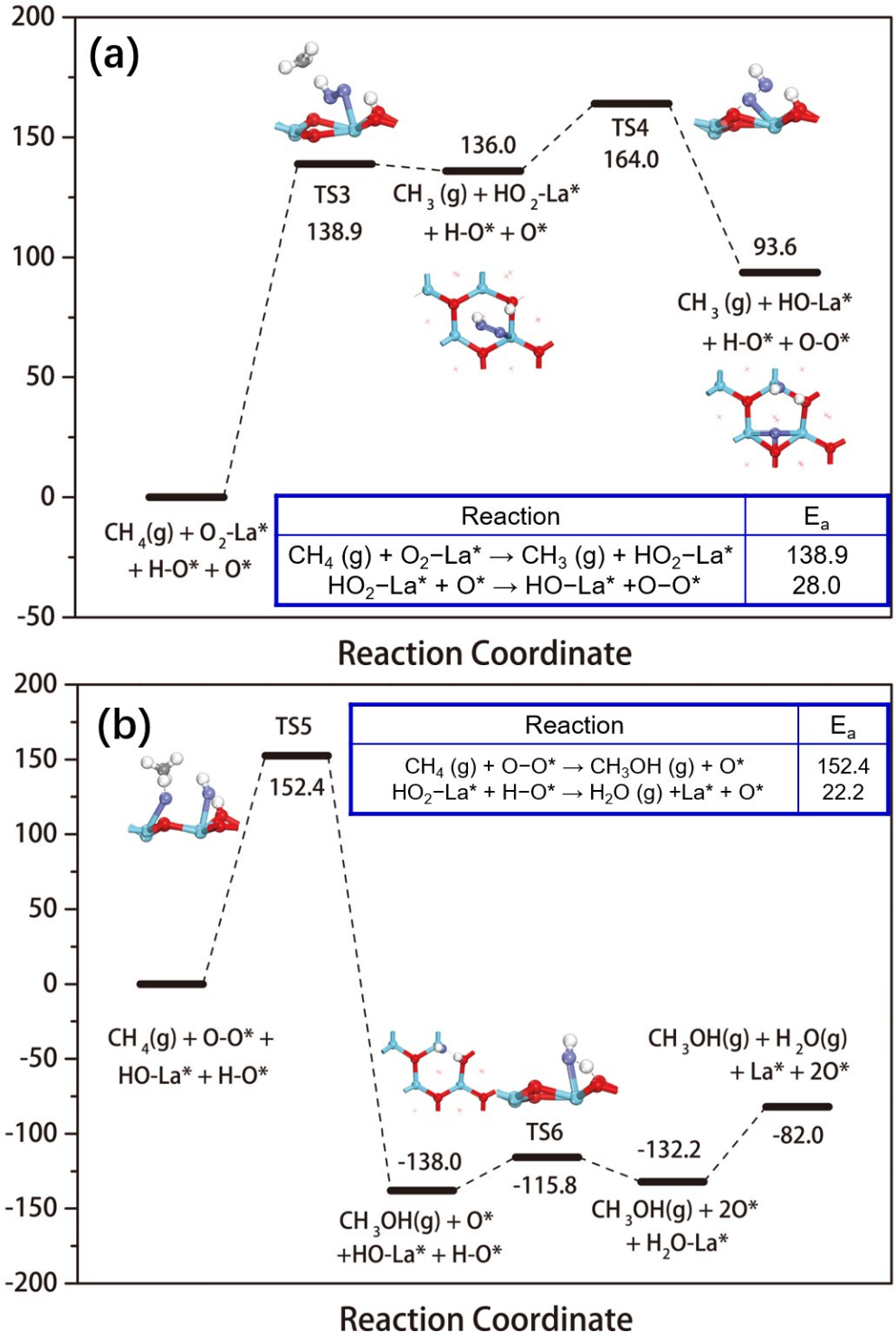

Figure S14. Potential energy surface (ΔE_{0K}, kJ/mol) for CH_3OH complete oxidation at the O_2^{2-} site on the $La_2O_3(001)$ surface. (a) CH_3OH oxidation and CH_2O formation. (b) CH_2O oxidation and HCOOH formation. (c) HCOOH oxidation and CO_2 formation. Dehydration of $CH_2(OH)_2$ and H_2CO_3 can occur directly (red) or with the H_2O assistance (black).

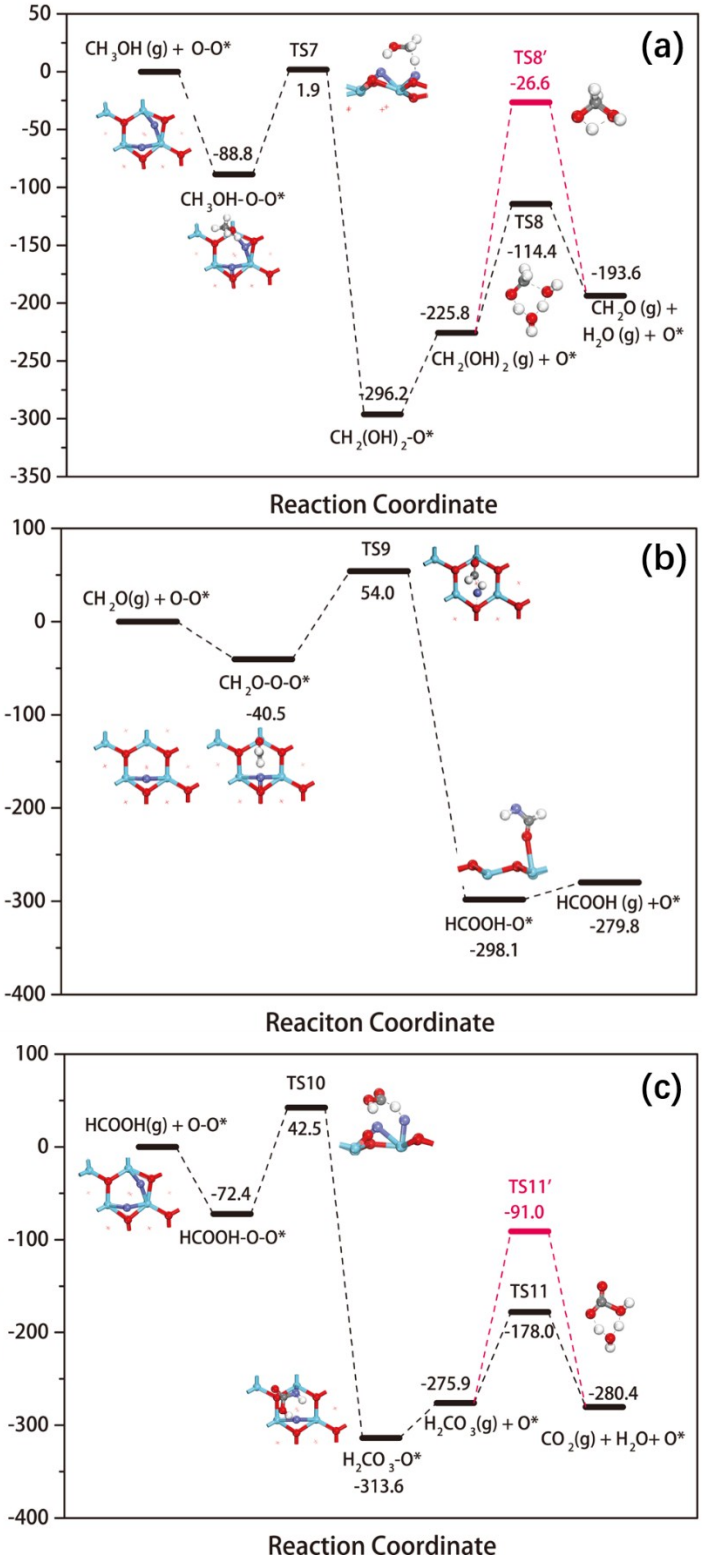

Table S1. Entropy (823K, J/mol*K) of gaseous molecules calculated by B3LYP, PBE, and Shomate equation.

Gas Molecule	B3LYP (J/mol*K)	PBE (J/mol*K)	EXP (J/mol*K)
H_2O	230.3	164.6	224.9[a]
CO_2	265.1	154.8	259.0[a]
CH_4	253.5	177.4	234.3[a]
CH_3·	256.8	177.9	240.5[a]
CH_3OH	300.1	200.8	299.0[b]
CH_2O	268.6	174.4	264.1[a]
O_2	239.2	137.5	236.9[a]
HCOOH	308.7	195.2	N/A
C_2H_6	319.9	217.7	305.9[b]
$CH_2(OH)_2$	341.0	503.0	N/A
$CH_2(OH)_2$+H_2O	445.2	319.2	N/A
CH_2O+2H_2O	489.1	368.9	N/A
CH_2O+H_2O	392.3	286.6	N/A
$CH_2(OH)_2$-ts	337.1	219.4	N/A
$CH_2(OH)_2$+H_2O -ts	412.4	280.5	N/A
H_2CO_3	348.8	221.7	N/A
H_2CO_3+H_2O	458.0	327.1	N/A
CO_2+H_2O	428.2	295.8	N/A
CO_2+2H_2O	518.2	381.9	N/A
H_2CO_3-ts	348.5	219.8	N/A
H_2CO_3+H_2O-ts	423.5	284.9	N/A

(a). P.J. Linstrom and W.G. Mallard, Eds., NIST Chemistry WebBook, NIST Standard Reference Database Number 69, National Institute of Standards and Technology, Gaithersburg MD, 20899.

(b). Haynes, W. M. (2009). CRC handbook of chemistry and physics: A ready-reference book of chemical and physical data. Boca Raton: CRC Press.

Table S2 Optimized fractional coordinates for structures shown in Figure S4.

Figure S4 (a): CH_4 physisorption on O_2^{2-}/La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   C    H
    25    16    1    4
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0042919689801878  0.0046869923828371  0.6208318011478569   T   T   T
  0.1658529173438485  0.3361183855405585  0.5350800043247905   T   T   T
  0.3196522178356225  0.1387596453551784  0.7123496080638548   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.9974523653963052  0.5046966752358806  0.6220828766723744   T   T   T
  0.1656424551699675  0.8300543703228289  0.5358066903893350   T   T   T
  0.3380253260304649  0.6754859039377631  0.6988976551374607   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.5049383026787166  0.0139491450313102  0.6191024601245458   T   T   T
  0.6701398477099937  0.3354321054815762  0.5337623094656189   T   T   T
  0.8368046951276072  0.1703684532394499  0.7059436943485902   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.4943953453886047  0.4777857986981134  0.6201180513643378   T   T   T
  0.6654489270484790  0.8320408190983687  0.5360509711020670   T   T   T
  0.8403058698712034  0.6756276838949020  0.7032188813897459   T   T   T
  0.4142292101326966  0.3296840629775110  0.7396309099125147   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1713011647858570  0.3383170134222270  0.6825503503221514   T   T   T
  0.3363904504995579  0.1695710075899829  0.5612918326579108   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1597087601017286  0.8222409361523281  0.6754443662534424   T   T   T
```

```
  0.3334777970946101  0.6660781946175115  0.5608284579693043   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6685603943924009  0.3393196030589416  0.6826766983833749   T   T   T
  0.8321887969577728  0.1670074962754008  0.5617371317555018   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6739682816213436  0.8411343634547487  0.6823624741349020   T   T   T
  0.8316767652001175  0.6644180889433150  0.5606033015710770   T   T   T
  0.2569207970861532  0.6028631628064026  0.8347736387404546   T   T   T
  0.2508809789040211  0.5973598061203887  0.8776155434120060   T   T   T
  0.1071305103445503  0.5288232251096697  0.8191560453033837   T   T   T
  0.3336931624179340  0.7560286397286718  0.8217984924158320   T   T   T
  0.3345711229295816  0.5290663369865826  0.8204190510968840   T   T   T
```

Figure S4 (a): Transition state for CH_4 activation on O_2^{2-}/La_2O_3 (001) surface

```
O   La   C   H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095201    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999999
   O   La   C   H
    25   16    1    4
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093740   F   F   F
  0.9782640017985057  0.9899862231536846  0.6209952368988482   T   T   T
  0.1673949789968183  0.3350670864333166  0.5367153978331112   T   T   T
  0.3245076164263903  0.1522680566173687  0.6980565805420353   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035880  0.8333092939980066  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093740   F   F   F
  0.9828174493881402  0.5039914628535341  0.6234871328950087   T   T   T
  0.1669087546819829  0.8349211806341006  0.5364420789133292   T   T   T
  0.3272443949246268  0.6749511267545886  0.7019464044016578   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468648  0.1666325478852855  0.4648237441093740   F   F   F
  0.5118665022605693  0.0019237711824985  0.6172804668754220   T   T   T
  0.6638959940157902  0.3331409844524048  0.5340078926014387   T   T   T
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  0.8323836195520578  0.1748729329985886  0.7074543017668852   T   T   T
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  0.6666870115944196  0.8333092939980066  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093740   F   F   F
  0.5084084755439299  0.5069704033071434  0.6202874870015854   T   T   T
  0.6641767162553091  0.8332918600729334  0.5334198043334851   T   T   T
  0.8313858039542832  0.6749005025209674  0.7090867399647220   T   T   T
  0.3884799492849512  0.3519259301022181  0.7556140504664710   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
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  0.3360251484288741  0.1692139482448924  0.5616441055492022   T   T   T
  0.1666222824035880  0.8333092939980066  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1478308029335392  0.8198088884121600  0.6772516783975214   T   T   T
  0.3372408640654857  0.6704807944141040  0.5609484818233186   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468648  0.1666325478852855  0.3192558875191267   F   F   F
  0.6676476019205470  0.3457527837059345  0.6843038954752971   T   T   T
  0.8288160000613595  0.1651862876385089  0.5615945549899132   T   T   T
  0.6666870115944196  0.8333092939980066  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6667938215311655  0.8434367005080506  0.6800701126329940   T   T   T
  0.8282960166465070  0.6661271884056799  0.5606962999681295   T   T   T
  0.4113319240116964  0.5515102326415642  0.8165291057466485   T   T   T
  0.4175098317560118  0.4709540534278894  0.8504081860196534   T   T   T
  0.2683176854200586  0.5343074195709120  0.8080214123506183   T   T   T
  0.5306543242124587  0.7043140157033785  0.8140555815350369   T   T   T
  0.4820645062530060  0.4945975285044845  0.7759953010771798   T   T   T
```

Figure S4 (a): CH_3OH adsorption on La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   C    H
    25    16    1    4
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0109273985085291 -0.0032194394516209  0.6214169999138275   T   T   T
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0.9999922729179431	0.5000441982274353	0.3790943669879780	F	F	F
0.1666222824035870	0.8333092939980062	0.2933258797492897	F	F	F
0.3333383730563639	0.6666767461127208	0.4648237441093741	F	F	F
-0.0006478227074990	0.5050991337024676	0.6195836271240680	T	T	T
0.1669780281319255	0.8321233110304664	0.5341231183602390	T	T	T
0.3387170202558819	0.6730718185254397	0.7021093107796973	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6665703570940948	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468647	0.1666325478852855	0.4648237441093741	F	F	F
0.4954920440163202	0.0072186862032795	0.6189488654530909	T	T	T
0.6688140483013906	0.3341813199687191	0.5344967968605746	T	T	T
0.8339087140545434	0.1660873857552096	0.7009636592990937	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.4994434029312040	0.4906875936552430	0.6218505722645187	T	T	T
0.6670315609950450	0.8339925644594073	0.5366521082918593	T	T	T
0.8329181779031132	0.6674940485825954	0.7055687541272504	T	T	T
0.2400823871952725	0.3108116570780692	0.7851268871681331	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1706623571256549	0.3382418686985061	0.6840722409717224	T	T	T
0.3337719363045051	0.1663678348950950	0.5612285632424163	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1667237909512652	0.8359395847056761	0.6800618845336417	T	T	T
0.3315356141017672	0.6667707318239938	0.5613002755674869	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6685254729953013	0.3352102470016728	0.6792587162466076	T	T	T
0.8338287277639487	0.1691188637614556	0.5612358863742429	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6709293812943627	0.8337334290831360	0.6794589303700804	T	T	T
0.8359834872282919	0.6664958666702938	0.5607576392342460	T	T	T
0.3806450204344870	0.4580907665672366	0.8191983368619070	T	T	T
0.5300098421591066	0.5283059991723441	0.8026422422815606	T	T	T
0.3820451483051778	0.3955634276909675	0.8576546211229257	T	T	T
0.3398601800722541	0.5713124077506779	0.8245605199735286	T	T	T
0.2988287161389750	0.2381009994390391	0.7668155629297384	T	T	T

Table S3. Optimized fractional coordinates for structures shown in Figure S1 & S12.

Figure S12 (a): clean La_2O_3 (001) surface

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La
    24    16
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.3333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.0000000000000000  0.0000000000000000  0.6206837706312953   T   T   T
  0.1666666666666714  0.3333333333333286  0.5352302760047607   T   T   T
  0.3333333333333286  0.1666666666666714  0.7050789635715589   T   T   T
  0.0000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.3333333333333357  0.6666666666666714  0.4648249768915562   F   F   F
  0.0000000000000000  0.5000000000000000  0.6206837706312953   T   T   T
  0.1666666666666714  0.8333333333333357  0.5352302760047607   T   T   T
  0.3333333333333357  0.6666666666666714  0.7050789635715589   T   T   T
  0.5000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.8333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.5000000000000000  0.0000000000000000  0.6206837706312953   T   T   T
  0.6666666666666714  0.3333333333333286  0.5352302760047607   T   T   T
  0.8333333333333286  0.1666666666666714  0.7050789635715589   T   T   T
  0.5000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.8333333333333286  0.6666666666666714  0.4648249768915562   F   F   F
  0.5000000000000000  0.5000000000000000  0.6206837706312953   T   T   T
  0.6666666666666714  0.8333333333333357  0.5352302760047607   T   T   T
  0.8333333333333286  0.6666666666666714  0.7050789635715589   T   T   T
  0.1666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.3333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.1666666666666714  0.3333333333333286  0.6810249590977548   T   T   T
  0.3333333333333286  0.1666666666666714  0.5612805770190477   T   T   T
  0.1666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.3333333333333357  0.6666666666666714  0.3192455779905217   F   F   F
  0.1666666666666714  0.8333333333333357  0.6810249590977548   T   T   T
```

```
  0.3333333333333357  0.6666666666666714  0.5612805770190477   T   T   T
  0.6666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.8333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.6666666666666714  0.3333333333333286  0.6810249590977548   T   T   T
  0.8333333333333286  0.1666666666666714  0.5612805770190477   T   T   T
  0.6666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.8333333333333286  0.6666666666666714  0.3192455779905217   F   F   F
  0.6666666666666714  0.8333333333333357  0.6810249590977548   T   T   T
  0.8333333333333286  0.6666666666666714  0.5612805770190477   T   T   T
```

Figure S9 (a): CH_4 physisorption on La_2O_3 (001)

```
C H  O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   C    H    O    La
     1    4    24    16
Selective dynamics
Direct
  0.5415234235982000  0.4367595237563628  0.8324847679637309   T   T   T
  0.6046544773101244  0.3695058294941468  0.8575348715984982   T   T   T
  0.4264497045096975  0.3235010953406744  0.8079009728128489   T   T   T
  0.4788016510667762  0.5057901216495189  0.8570073628540872   T   T   T
  0.6568326144237462  0.5482479223704261  0.8075582890793367   T   T   T
  0.0000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.3333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
 -0.0004713765953101  0.0000827461058967  0.6203185653540269   T   T   T
  0.1668108112612808  0.3334666582502842  0.5351401647216484   T   T   T
  0.3324590529912619  0.1660792890033372  0.7046808494937937   T   T   T
  0.0000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.3333333333333357  0.6666666666666714  0.4648249768915562   F   F   F
 -0.0003120628015060  0.4996285742607460  0.6205314781933086   T   T   T
  0.1666980570482100  0.8333030640191692  0.5351884213404017   T   T   T
  0.3333162923610548  0.6666685132631236  0.7046895384824261   T   T   T
  0.5000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.8333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.5004175516143455  0.0002365099692532  0.6205032384744323   T   T   T
  0.6665854966288095  0.3333815670825416  0.5350817180368599   T   T   T
  0.8331314546883252  0.1668982221992416  0.7049060686142941   T   T   T
  0.5000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
```

```
  0.6666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.8333333333333286  0.6666666666666714  0.4648249768915562   F   F   F
  0.5001230755213972  0.4999384178267055  0.6205746468422124   T   T   T
  0.6665108595375658  0.8331771731970579  0.5351199107788950   T   T   T
  0.8335219666309313  0.6671172312467939  0.7048626902001714   T   T   T
  0.1666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.3333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.1663608858895003  0.3334914554131782  0.6806781450148104   T   T   T
  0.3334883944231191  0.1668057043334014  0.5611977820670250   T   T   T
  0.1666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.3333333333333357  0.6666666666666714  0.3192455779905217   F   F   F
  0.1665144348694414  0.8330816251613603  0.6805891628254079   T   T   T
  0.3333935616690131  0.6666682405701693  0.5611067227027053   T   T   T
  0.6666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.8333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.6663472525465187  0.3334314726116776  0.6811750585073364   T   T   T
  0.8332187344945178  0.1666994483897120  0.5612138156908103   T   T   T
  0.6666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.8333333333333286  0.6666666666666714  0.3192455779905217   F   F   F
  0.6665169281954451  0.8335563809336630  0.6807145379915591   T   T   T
  0.8331569246709593  0.6665206561200220  0.5611837047266295   T   T   T
```

Figure S12 (a): Transition state for CH_4 activation on La_2O_3 (001)

```
C H  O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095201    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999999
   C    H    O    La
     1    4   24   16
Selective dynamics
Direct
  0.5062210425165201  0.4148650041650212  0.7719394015511107   T   T   T
  0.3480274223232149  0.3089967326586339  0.7785654374387178   T   T   T
  0.5308201703126473  0.5483113644749329  0.7929255906450031   T   T   T
  0.5776456947845601  0.3534322751505139  0.7971724634631447   T   T   T
  0.7786860502439676  0.6381747798788042  0.7515427316723150   T   T   T
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093740   F   F   F
  0.9457173388472709  0.9658033849058493  0.6189301079893460   T   T   T
  0.1689681384200261  0.3323241331323897  0.5393122502260245   T   T   T
  0.3260253637991373  0.1645503844600424  0.6718059584165869   T   T   T
  0.9999897345183015  0.5000441982274353  0.3790943669879780   F   F   F
```

0.1666222824035872	0.8333092939980066	0.2933258797492897	F	F	F
0.3333383730563639	0.6666767461127208	0.4648237441093740	F	F	F
0.9991368435444780	0.5207818946556539	0.6268313600678752	T	T	T
0.1714915318780432	0.8394283876422274	0.5377425271288422	T	T	T
0.3303767678237060	0.6786125306649332	0.7080747549048046	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6666972770761177	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468619	0.1666325478852855	0.4648237441093740	F	F	F
0.5148969415061350	0.9749214362708853	0.6199182728046803	T	T	T
0.6604713470154632	0.3283034461687344	0.5380457104758701	T	T	T
0.8399468962679478	0.1873038413795438	0.7066430237881718	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944197	0.8333092939980066	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093740	F	F	F
0.5375284741424655	0.5486390086522397	0.6235910316585707	T	T	T
0.6640647386081098	0.8344509569166144	0.5306346859914319	T	T	T
0.8683986835774096	0.7021203300125245	0.7218168989500722	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1748534567865996	0.3530654621558307	0.6868786306933942	T	T	T
0.3333998462971989	0.1665951747949214	0.5640148707857244	T	T	T
0.1666222824035872	0.8333092939980066	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1699673018086395	0.8268047844996611	0.6754056236171864	T	T	T
0.3415900236803753	0.6720614610314651	0.5605887465497611	T	T	T
0.6666972770761177	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468619	0.1666325478852855	0.3192558875191267	F	F	F
0.6651980604989709	0.3450286798495747	0.6831611180932826	T	T	T
0.8284669345437016	0.1580228715939993	0.5619542773096086	T	T	T
0.6666870115944197	0.8333092939980066	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6673076863872720	0.8473681481337767	0.6804947507620317	T	T	T
0.8287289562387530	0.6711285857211691	0.5614159497043710	T	T	T

Figure S12 (a): CH_4 chemisorption on La_2O_3 (001)

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   C    H
    24    16    1    4
Selective dynamics
Direct
```

0.0000000000000000	0.0000000000000000	0.3790754283204265	F	F	F
0.1666666666666714	0.3333333333333286	0.2933258797492897	F	F	F
0.3333333333333286	0.1666666666666714	0.4648249768915562	F	F	F
-0.0557187946791243	-0.0425192828899778	0.6206341749171792	T	T	T
0.1689414849563295	0.3337575442400762	0.5398388154231940	T	T	T
0.3330263582002418	0.1607351186601873	0.6692549037614668	T	T	T
0.0000000000000000	0.5000000000000000	0.3790754283204265	F	F	F
0.1666666666666714	0.8333333333333357	0.2933258797492897	F	F	F
0.3333333333333357	0.6666666666666714	0.4648249768915562	F	F	F
-0.0320480155862292	0.5159912927887869	0.6269983176029640	T	T	T
0.1740156317791328	0.8391377692457254	0.5396813776927935	T	T	T
0.3283191810718461	0.6793984525603312	0.7047132214330397	T	T	T
0.5000000000000000	0.0000000000000000	0.3790754283204265	F	F	F
0.6666666666666714	0.3333333333333286	0.2933258797492897	F	F	F
0.8333333333333286	0.1666666666666714	0.4648249768915562	F	F	F
0.5280762726212179	-0.0184144317276230	0.6198303867186902	T	T	T
0.6595677171980721	0.3265459060582704	0.5365305579458544	T	T	T
0.8442657488967621	0.1842940601679177	0.7089390562256936	T	T	T
0.5000000000000000	0.5000000000000000	0.3790754283204265	F	F	F
0.6666666666666714	0.8333333333333357	0.2933258797492897	F	F	F
0.8333333333333286	0.6666666666666714	0.4648249768915562	F	F	F
0.5315385534904071	0.5468827819287075	0.6225585505882822	T	T	T
0.6648821795993197	0.8355102890300824	0.5304490986757231	T	T	T
0.8697686607219817	0.6955927903768955	0.7242797083838656	T	T	T
0.1666666666666714	0.3333333333333286	0.4389052786503242	F	F	F
0.3333333333333286	0.1666666666666714	0.3192455779905217	F	F	F
0.1903036661686536	0.3498832900549255	0.6905929067928133	T	T	T
0.3360160599369844	0.1695716222108016	0.5641539528699624	T	T	T
0.1666666666666714	0.8333333333333357	0.4389052786503242	F	F	F
0.3333333333333357	0.6666666666666714	0.3192455779905217	F	F	F
0.1668511301900182	0.8244623715368173	0.6721538213178333	T	T	T
0.3471261500604420	0.6730008045416582	0.5606858878401115	T	T	T
0.6666666666666714	0.3333333333333286	0.4389052786503242	F	F	F
0.8333333333333286	0.1666666666666714	0.3192455779905217	F	F	F
0.6724330642542042	0.3407653811705439	0.6840394968147782	T	T	T
0.8282312920295005	0.1588803360246177	0.5622315506693398	T	T	T
0.6666666666666714	0.8333333333333357	0.4389052786503242	F	F	F
0.8333333333333286	0.6666666666666714	0.3192455779905217	F	F	F
0.6692106007703873	0.8459098981277162	0.6809524555436887	T	T	T
0.8274470848667121	0.6679986719363669	0.5614955073961316	T	T	T
0.4627619656447258	0.4078414399168034	0.7686055882926845	T	T	T
0.3187657203484952	0.3166967891560279	0.7885670388019231	T	T	T
0.5208823218129955	0.5531963475571090	0.7873700806516003	T	T	T
0.5503519675456348	0.3462264788902113	0.7859868278989690	T	T	T

0.8384042739296932 0.6757661570768696 0.7613849994396908 T T T

Figure S12 (a): CH_3 desorption from La_2O_3 (001)

```
H O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   H    O    La
     1    24    16
Selective dynamics
Direct
  0.8334805838559880  0.6668478244591235  0.7637305480867156   T   T   T
  0.0000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.3333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.9877125329117543  0.9754698988410706  0.6248475498161034   T   T   T
  0.1666729674848583  0.3333415645404568  0.5359866318787792   T   T   T
  0.3325917005050004  0.1673141138553516  0.7052039080418606   T   T   T
  0.0000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.3333333333333357  0.6666666666666714  0.4648249768915562   F   F   F
  0.9875940156784582  0.5121864109314733  0.6248363540009830   T   T   T
  0.1686696468817887  0.8343311807276962  0.5354622977775434   T   T   T
  0.3325766532452330  0.6651886368409275  0.7051709543742907   T   T   T
  0.5000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.8333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.4999929711755242 -0.0000028049852987  0.6239661921429885   T   T   T
  0.6656601835604030  0.3313266129550522  0.5354485468143212   T   T   T
  0.8346750993209026  0.1673030839685538  0.7052185442608401   T   T   T
  0.5000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.8333333333333286  0.6666666666666714  0.4648249768915562   F   F   F
  0.5246246589411742  0.5122518278089314  0.6248315167372052   T   T   T
  0.6656679714308961  0.8343395807711003  0.5354582716150054   T   T   T
  0.8333644761726083  0.6667047845996544  0.7256104897272919   T   T   T
  0.1666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.3333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.1665733053208846  0.3332168897590834  0.6828542484513703   T   T   T
  0.3345219021217783  0.1655032626477846  0.5608217132279144   T   T   T
  0.1666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.3333333333333357  0.6666666666666714  0.3192455779905217   F   F   F
  0.1748232897546233  0.8373954101490578  0.6798367674136132   T   T   T
```

```
  0.3345224069268751  0.6690263997022076  0.5608213085962328   T   T   T
  0.6666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.8333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.6625750519056584  0.3251665250438564  0.6798527077523208   T   T   T
  0.8309865060369082  0.1655096213889894  0.5608219560718776   T   T   T
  0.6666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.8333333333333286  0.6666666666666714  0.3192455779905217   F   F   F
  0.6625547233025123  0.8373791663198332  0.6798420559802251   T   T   T
  0.8333161698154112  0.6666448105779532  0.5623238184066305   T   T   T
```

Figure S12 (b): O_2 physisorption on CH_3/La_2O_3 (001)

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   C    H
    26    16    1    4
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.9425655087001364  0.9553045066248074  0.6210783765760317   T   T   T
  0.1682493394003557  0.3330992394299409  0.5400018767531444   T   T   T
  0.3305708810846925  0.1584830911380148  0.6691780084027138   T   T   T
  0.9999897345183015  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.9648254560418923  0.5136061661627821  0.6271901455485561   T   T   T
  0.1731076237236177  0.8382935645955086  0.5398231792286468   T   T   T
  0.3254471316946541  0.6766337429569580  0.7042139403398151   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.5273558003820530  0.9813292624469914  0.6197519246917869   T   T   T
  0.6589702141360175  0.3258168138904031  0.5364678979481601   T   T   T
  0.8413303101537781  0.1814258653322298  0.7087075202627303   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.5308658780035129  0.5454446862463694  0.6224414967394069   T   T   T
  0.6643875475638240  0.8351118948476839  0.5305017087748887   T   T   T
  0.8642962842014695  0.6901969592342154  0.7244887352383539   T   T   T
```

0.8326105717442902 0.3958299075980026 0.8932894418005015 T T T
0.8363378990182653 0.4251906396535716 0.8456012314008450 T T T
0.1666325478852855 0.3332650957705710 0.4388937363395371 F F F
0.3333486385380624 0.1666325478852855 0.3192558875191267 F F F
0.1858665678717074 0.3466151575216218 0.6904425856368925 T T T
0.3355613060506093 0.1688481104752509 0.5641971759736651 T T T
0.1666222824035870 0.8333092939980062 0.4388937363395371 F F F
0.3333383730563639 0.6666767461127208 0.3192558875191267 F F F
0.1631875438992489 0.8220602452972300 0.6724319500747826 T T T
0.3466146875195715 0.6725557393825519 0.5606981362186115 T T T
0.6665703570940948 0.3332650957705710 0.4388937363395371 F F F
0.8332864477468647 0.1666325478852855 0.3192558875191267 F F F
0.6698270206885881 0.3376401413239759 0.6839126451799178 T T T
0.8273647277910221 0.1582647105521994 0.5622202818526029 T T T
0.6666870115944192 0.8333092939980062 0.4388937363395371 F F F
0.8332761822651662 0.6666767461127208 0.3192558875191267 F F F
0.6664893504461938 0.8432923018607754 0.6808890106080322 T T T
0.8263925137799893 0.6669875215115124 0.5614743721543494 T T T
0.4523080225755766 0.4001413478857802 0.7693426503393640 T T T
0.3091176057670607 0.3122678829059610 0.7898190193443327 T T T
0.5166818746279486 0.5461960861573957 0.7878388286972775 T T T
0.5382266613942305 0.3338906241931578 0.7847322222025249 T T T
0.8388265316581763 0.6713053999575511 0.7619236392888825 T T T

Figure S12 (b): transition state for O_2 chemisorption on CH_3/La_2O_3 (001)

O La C H
1.00000000000000
7.8789800000000003 0.0000000000000000 0.0000000000000000
-3.9394900000000002 6.8233968359095201 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5688315207999999
O La C H
26 16 1 4
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.3790943669879780 F F F
0.1666325478852855 0.3332650957705710 0.2933258797492897 F F F
0.3333486385380624 0.1666325478852855 0.4648237441093741 F F F
0.9385684955860633 0.9533548689159038 0.6222832608816901 T T T
0.1676958381409931 0.3337574466357362 0.5405254906160644 T T T
0.3265792977506040 0.1577173117812783 0.6685069371259494 T T T
0.9999922729179431 0.5000441982274353 0.3790943669879780 F F F
0.1666222824035870 0.8333092939980062 0.2933258797492897 F F F
0.3333383730563639 0.6666767461127208 0.4648237441093741 F F F

0.9528574954723306	0.5102713309792770	0.6278888375205631	T	T	T
0.1712345238494736	0.8377118469816981	0.5402163544286537	T	T	T
0.3176893077289566	0.6769548134839473	0.7009311822341870	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6665703570940948	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468647	0.1666325478852855	0.4648237441093741	F	F	F
0.5281126378104330	0.9870681750057816	0.6184841986109806	T	T	T
0.6586231949391087	0.3265700094798543	0.5356259609407718	T	T	T
0.8318555381858376	0.1780236696479267	0.7087439411864569	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.5290810474657256	0.5449403075393937	0.6217542538771080	T	T	T
0.6635284071678172	0.8356101077768178	0.5304533598561658	T	T	T
0.8489592042710821	0.6828262676269411	0.7252025700424772	T	T	T
0.7209305242983531	0.3768575196469497	0.8756955293557629	T	T	T
0.7970415369533772	0.4065750529138823	0.8317745879968145	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1747966512482252	0.3436213221227006	0.6884497020782641	T	T	T
0.3363762530213677	0.1692767487723800	0.5641649716267894	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1517306032199555	0.8219279880058731	0.6727253095635294	T	T	T
0.3463241568052186	0.6737554344215118	0.5608476862312154	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6633877682415626	0.3347720101863134	0.6838534498142504	T	T	T
0.8258037853149728	0.1590904744547054	0.5619543396323472	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6590464724725725	0.8421734922444011	0.6805093790917727	T	T	T
0.8237567891644904	0.6662652539324320	0.5613696451916410	T	T	T
0.3982448915646052	0.3829713331725534	0.7715924095286812	T	T	T
0.2533707495610668	0.3088189289648914	0.7918813419469944	T	T	T
0.4787673167291454	0.5272904218424679	0.7909512336465200	T	T	T
0.4664639212325410	0.2969412468255303	0.7847487872619918	T	T	T
0.8319260522325501	0.6673798500131906	0.7629710131270864	T	T	T

Figure S9 (b): superoxide site on H/La_2O_3 (001)

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
```

0.0000000000000000 0.0000000000000000 25.5688315207999963

O La H

26 16 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.3790943669879780	F	F	F
0.1666325478852855	0.3332650957705710	0.2933258797492897	F	F	F
0.3333486385380624	0.1666325478852855	0.4648237441093741	F	F	F
0.9400696486672429	0.9579057404184601	0.6202757685706384	T	T	T
0.1668563621334901	0.3313959387699106	0.5400474352925920	T	T	T
0.3227352265714042	0.1603944287854308	0.6685607765069449	T	T	T
0.9999897345183015	0.5000441982274353	0.3790943669879780	F	F	F
0.1666222824035870	0.8333092939980062	0.2933258797492897	F	F	F
0.3333383730563639	0.6666767461127208	0.4648237441093741	F	F	F
0.9831224060602163	0.5115530512372033	0.6283847256111950	T	T	T
0.1712992903950515	0.8380463780390651	0.5391545353134843	T	T	T
0.3232108842286886	0.6734229991737640	0.7060411300829885	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6665703570940948	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468647	0.1666325478852855	0.4648237441093741	F	F	F
0.5176506773332225	0.9763513676975678	0.6200089301601360	T	T	T
0.6601684619410547	0.3267013881519686	0.5372192859953214	T	T	T
0.8371083280330686	0.1779714355372840	0.7069426963185073	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.5328978953786416	0.5489575453018165	0.6214689595442455	T	T	T
0.6641376390133310	0.8344415830204959	0.5303803155576613	T	T	T
0.8612262292386937	0.6916966173517346	0.7236549364250318	T	T	T
0.5295589070754061	0.3118719048372247	0.7755312895357919	T	T	T
0.4524143708820145	0.4125515890813980	0.7530405126653719	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1660803304853472	0.3457827067830774	0.6858037610353016	T	T	T
0.3349475821200910	0.1678238836107761	0.5644023225809688	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1662282040025024	0.8240316370177653	0.6735847630014550	T	T	T
0.3439433704217996	0.6713288594933103	0.5604885841265875	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6623024627260876	0.3371131996048397	0.6848735746118977	T	T	T
0.8263463083938579	0.1565457394928068	0.5620378120604919	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F

0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6621214922579070	0.8402968649956096	0.6806382303572067	T	T	T
0.8264137529576869	0.6682044447803462	0.5614950929305366	T	T	T
0.8361890894153027	0.6678806374274904	0.7610057345584271	T	T	T

Table S4. Optimized fractional coordinates for structures shown in Figure S2 & S13.

Figure S13 (a): CH_4 physisorption on O_2^-/H/La_2O_3 (001)

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   C    H
    26    16    1    5
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.9438608932258923  0.9600190592706944  0.6200047934207665   T   T   T
  0.1682346986382908  0.3321672247192209  0.5396993951053601   T   T   T
  0.3262386326875681  0.1627371284492753  0.6697460621014319   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.9856514265833575  0.5112087799049033  0.6281371329567160   T   T   T
  0.1730187760558694  0.8389380378507905  0.5393819326558283   T   T   T
  0.3278224819428322  0.6754596090420272  0.7055978381710100   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.5211389905328336  0.9790972942620579  0.6202911063809246   T   T   T
  0.6609423453719621  0.3273940823721715  0.5371323708487403   T   T   T
  0.8404590821968468  0.1785653911110167  0.7072536427372150   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.5347499760399689  0.5494795934155419  0.6210165925952621   T   T   T
  0.6650715847683505  0.8351555735042085  0.5303600458926462   T   T   T
  0.8682539518577916  0.6956653516429605  0.7232487882927247   T   T   T
  0.5444506968488142  0.3261565985502850  0.7759095569797014   T   T   T
  0.4650428745250840  0.4231905379588736  0.7524945343948751   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1698200633374725  0.3474799188659136  0.6863712501868307   T   T   T
  0.3360979567965353  0.1691748574085853  0.5643256554177025   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
```

```
  0.1711524575235679  0.8264631739354701  0.6730347861804956   T   T   T
  0.3452058937883893  0.6716052738252754  0.5605224301784990   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6672202744653312  0.3387490100536879  0.6846588427326362   T   T   T
  0.8277616341877952  0.1576722004126502  0.5620354879160808   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6661419457660548  0.8414795252281435  0.6807000414914179   T   T   T
  0.8276563459795240  0.6689750873683832  0.5614113217764465   T   T   T
  0.1296024006058684  0.4348178360248217  0.8513102892630036   T   T   T
  0.8427579565254852  0.6698228444880382  0.7605102852355461   T   T   T
  0.2548164444398352  0.4378676248884230  0.8316890144705908   T   T   T
 -0.0073918479066749  0.3272348109156942  0.8323311539924252   T   T   T
  0.1266076221354935  0.3943801517479499  0.8924625776357867   T   T   T
  0.1442455418084733  0.5805355899488879  0.8490081920390651   T   T   T
```

Figure S13 (a): transition state for CH_4 activation on O_2^-/H/La_2O_3 (001)

```
O   La   C   H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095201    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999999
   O   La   C   H
    26   16    1    5
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093740   F   F   F
  0.9439869973636790  0.9593347675929838  0.6194161113513221   T   T   T
  0.1672445484857085  0.3301145847762986  0.5387875496960478   T   T   T
  0.3237655967359762  0.1622940627498567  0.6723710333367190   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035872  0.8333092939980066  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093740   F   F   F
  0.9901503074264686  0.5025372243270626  0.6259111168015515   T   T   T
  0.1699439993432569  0.8373055663977191  0.5388525815251798   T   T   T
  0.3195480317124885  0.6735378270314593  0.7056450148919720   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468619  0.1666325478852855  0.4648237441093740   F   F   F
  0.5193888569448477  0.9809335654439014  0.6204339746390951   T   T   T
```

```
  0.6593696148919396  0.3267143125827133  0.5369917016441709   T   T   T
  0.8373969728066667  0.1708877264373037  0.7072406404807413   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944197  0.8333092939980066  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093740   F   F   F
  0.5249876022009428  0.5452546413260008  0.6204303733101015   T   T   T
  0.6634165498134846  0.8333434405914731  0.5302127992305957   T   T   T
  0.8618607021124389  0.6900858885930142  0.7195884751319694   T   T   T
  0.5806295729097779  0.3745769979995169  0.7708163572330732   T   T   T
  0.4665155416895414  0.4677263920291930  0.7561321941944759   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1653691617120760  0.3449835312253879  0.6823344807480574   T   T   T
  0.3341360744664277  0.1670407620922579  0.5637034455882095   T   T   T
  0.1666222824035872  0.8333092939980066  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1641960657579104  0.8244138190096092  0.6729036997517752   T   T   T
  0.3417619789016794  0.6695110931914149  0.5603577065912294   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468619  0.1666325478852855  0.3192558875191267   F   F   F
  0.6647572424339120  0.3238241010233713  0.6831471506506273   T   T   T
  0.8267729809542524  0.1562822503673358  0.5617995934994344   T   T   T
  0.6666870115944197  0.8333092939980066  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6595279206072663  0.8322881384749009  0.6816609559382913   T   T   T
  0.8250826656794065  0.6676927332464492  0.5611541751919268   T   T   T
  0.2384964254435901  0.4330560052406881  0.8381512451088735   T   T   T
  0.8007138516834607  0.6174996458547469  0.7522733557387640   T   T   T
  0.3884486200161142  0.4635974598209220  0.7903033299835952   T   T   T
  0.0945512889893869  0.3217429823327227  0.8239176279248859   T   T   T
  0.3145963875998291  0.3851677858776981  0.8648105494133140   T   T   T
  0.2639721869496247  0.5817312783654484  0.8423752396545384   T   T   T
```

Figure S13 (a): CH_4 chemisorption on $O_2^-/H/La_2O_3$ (001)

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O   La   C   H
   26   16    1    5
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
```

0.1666325478852855	0.3332650957705710	0.2933258797492897	F	F	F
0.3333486385380624	0.1666325478852855	0.4648237441093741	F	F	F
0.9465792754266584	0.9625385338934608	0.6193047725148340	T	T	T
0.1687506289017429	0.3312386796782510	0.5387704311116043	T	T	T
0.3277148699425044	0.1648913206751405	0.6738299000000258	T	T	T
0.9999922729179431	0.5000441982274353	0.3790943669879780	F	F	F
0.1666222824035870	0.8333092939980062	0.2933258797492897	F	F	F
0.3333383730563639	0.6666767461127208	0.4648237441093741	F	F	F
-0.0061662818636753	0.5023807922284399	0.6264604062150957	T	T	T
0.1713484328180201	0.8386850105435715	0.5391330354044630	T	T	T
0.3218350066491928	0.6757308674144075	0.7067644374922514	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6665703570940948	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468647	0.1666325478852855	0.4648237441093741	F	F	F
0.5218628866074667	0.9825511767923060	0.6209718690913676	T	T	T
0.6607499788516742	0.3283202879285591	0.5371776692145497	T	T	T
0.8399800464992956	0.1727178677134719	0.7082044500950834	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.5256566607508629	0.5467169545854191	0.6206322859242890	T	T	T
0.6647631824180489	0.8341553094248272	0.5304178121547900	T	T	T
0.8675559260914155	0.6958301207832138	0.7196067183356918	T	T	T
0.5935386789475332	0.3877886692439435	0.7719098618336288	T	T	T
0.4760743962271472	0.4787743541395890	0.7549385127739738	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1680028038271812	0.3472941273563950	0.6828984381405211	T	T	T
0.3356497093683816	0.1688496514369485	0.5638034450106257	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1679879393702540	0.8270458688077584	0.6731699195167041	T	T	T
0.3431784772193953	0.6703282922944103	0.5606506776766740	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6682838271302760	0.3260996935978068	0.6840991992906383	T	T	T
0.8282410013163547	0.1575004298433900	0.5621005917747540	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6623856867563845	0.8338510715273033	0.6820460840627355	T	T	T
0.8266854954736872	0.6693292066342584	0.5612921517523388	T	T	T
0.2328046067662680	0.4577935537846037	0.8468231906631385	T	T	T
0.8040546092091526	0.6190379472261289	0.7518633951491639	T	T	T
0.4185246575199946	0.4916048337811472	0.7884480185971589	T	T	T

```
  0.0904531129453206  0.3497046399927971  0.8313769894903755   T   T   T
  0.3193458190897355  0.4089202522238922  0.8685835161248293   T   T   T
  0.2703305726777188  0.6105710138785135  0.8485795491340623   T   T   T
```

Figure S13 (a): CH_3 desorption and OOH on H/La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   H
    26    16    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.9466861840003770  0.9611832552012952  0.6191503609132947   T   T   T
  0.1676728774095434  0.3304852415697402  0.5388766024270811   T   T   T
  0.3271598987026028  0.1656436742900451  0.6735333810725470   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.9993086391554843  0.5099271780613217  0.6271488151329719   T   T   T
  0.1710114722453311  0.8388891867573990  0.5383670913988498   T   T   T
  0.3255914404877430  0.6777815647174441  0.7087199678214904   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.5182042168397374  0.9798055820911600  0.6208915233249006   T   T   T
  0.6608035639255084  0.3278242918819300  0.5377233597457599   T   T   T
  0.8397684117361827  0.1746447730068144  0.7066748635850205   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.5253364530940672  0.5477067773108824  0.6207938445446936   T   T   T
  0.6647700648006087  0.8343858899211394  0.5304919739305755   T   T   T
  0.8634553021888381  0.6945823309139697  0.7203921731158917   T   T   T
  0.5896137676776606  0.3767010101661274  0.7725096388799070   T   T   T
  0.4618552889886828  0.4574199267001196  0.7560061854863361   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1695096768221500  0.3498350681514242  0.6838243750355266   T   T   T
  0.3343970864525274  0.1675629374816516  0.5640647029645628   T   T   T
```

```
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1693924336339536  0.8275069316717805  0.6749669391681863   T   T   T
  0.3418940874364798  0.6701969210424916  0.5605769513103557   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6678946421397752  0.3287681429989523  0.6839397377083710   T   T   T
  0.8281750149894402  0.1569776005840792  0.5618441239504692   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6635550674757618  0.8364323882012428  0.6808126872423318   T   T   T
  0.8275344510803532  0.6697204197149283  0.5612753496344051   T   T   T
  0.8028254251274547  0.6164968925916315  0.7525402030661691   T   T   T
  0.4678118478522577  0.5350411476748632  0.7864914759597315   T   T   T
```

Figure S13 (a): transition state for OOH dissociation on H/La_2O_3 (001) surface

```
O   La   H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095201    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999999
   O   La   H
    26   16    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093740   F   F   F
  0.0000365549791633  0.9778060565569483  0.6249731656911571   T   T   T
  0.1672209801382986  0.3353279089971135  0.5380541314406481   T   T   T
  0.3307800578354401  0.1415576847200303  0.7094251777389370   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035880  0.8333092939980066  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093740   F   F   F
  0.9713954993124994  0.5012783937916765  0.6204729877346444   T   T   T
  0.1722055376108053  0.8320831542383279  0.5362908670880510   T   T   T
  0.3360821195558930  0.6649309466723510  0.6894733839487659   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468648  0.1666325478852855  0.4648237441093740   F   F   F
  0.5082638235981278  0.0230442418057558  0.6197250638164162   T   T   T
  0.6676382356436843  0.3296366779773381  0.5322228804646512   T   T   T
  0.8394631060474966  0.1543250695300985  0.7063305248790016   T   T   T
```

```
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944196  0.8333092939980066  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093740   F   F   F
  0.5229907550663787  0.4844342131270788  0.6212318402351862   T   T   T
  0.6633316115251123  0.8335703799597489  0.5362856824234780   T   T   T
  0.8772244973999327  0.6651833149649319  0.7200913099476063   T   T   T
  0.4630138359742098  0.3961010089824918  0.7430164179892337   T   T   T
  0.5984726354886711  0.6456547711259404  0.7746634997150748   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1812375308887181  0.3254231855348911  0.6865788302474342   T   T   T
  0.3414153464538351  0.1698599794877211  0.5607805305787520   T   T   T
  0.1666222824035880  0.8333092939980066  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1756628670129969  0.8323927341959332  0.6730681597670184   T   T   T
  0.3361182745118328  0.6669796489446249  0.5617456948810531   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468648  0.1666325478852855  0.3192558875191267   F   F   F
  0.6692494800326825  0.3236454753001364  0.6825295116728454   T   T   T
  0.8295879862045079  0.1669674145283196  0.5624908864086089   T   T   T
  0.6666870115944196  0.8333092939980066  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6714590396595667  0.8226561360501200  0.6889041021751592   T   T   T
  0.8308836964506803  0.6610678949626201  0.5615786669556190   T   T   T
  0.5199005423559764  0.6023039518604077  0.8062723934381639   T   T   T
  0.8087721132945214  0.6497406173407592  0.7539271034617003   T   T   T
```

Figure S13 (a): peroxide site on OH/H/La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   H
    26    16    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0168568090783988 -0.0134015482721804  0.6236489876135516   T   T   T
  0.1619587015322523  0.3375591218741149  0.5387475471748869   T   T   T
  0.3245912627578681  0.1348335466775966  0.7158176155512872   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
```

0.1666222824035870	0.8333092939980062	0.2933258797492897	F	F	F
0.3333383730563639	0.6666767461127208	0.4648237441093741	F	F	F
-0.0220635831399763	0.5223997374321017	0.6213036107220093	T	T	T
0.1677586882317174	0.8297483229762359	0.5340496910173484	T	T	T
0.3343134915063860	0.6641696534847573	0.6911959630395321	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6665703570940948	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468647	0.1666325478852855	0.4648237441093741	F	F	F
0.4910375145307025	0.0188813300657668	0.6189144508677245	T	T	T
0.6700456329261553	0.3319142384773739	0.5328482191862266	T	T	T
0.8450114047377025	0.1762800855664199	0.6971372540474329	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.5073257698301329	0.4667229353118880	0.6223294528381993	T	T	T
0.6628692895455983	0.8356538304932650	0.5371254564196344	T	T	T
0.8612859041305457	0.6581854835282018	0.7202784276398699	T	T	T
0.4192785407788511	0.3299565380705151	0.7408807721016956	T	T	T
0.6984659781265207	0.8081040721030295	0.7786794744179885	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1794628090986139	0.3291548796169704	0.6821509794035120	T	T	T
0.3365401881861470	0.1674445336150903	0.5608666571551860	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1680989504029423	0.8268417093979717	0.6745697633654177	T	T	T
0.3330005832307488	0.6708164809120681	0.5615077910922657	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6654948642959131	0.3316597384402453	0.6807151737752176	T	T	T
0.8268828216321805	0.1667831158351291	0.5625587146455246	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6719654262780124	0.8381648391598967	0.6932236541982327	T	T	T
0.8318427943723440	0.6644193826848652	0.5610386470387581	T	T	T
0.6473852186002336	0.7889019324560380	0.8139213420223457	T	T	T
0.8184721014521734	0.6878606104858582	0.7544112432722485	T	T	T

Figure S13 (b): CH_4 physisorption on O_2^{2-}

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
```

O La H C

26 16 6 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.3790943669879780	F	F	F
0.1666325478852855	0.3332650957705710	0.2933258797492897	F	F	F
0.3333486385380624	0.1666325478852855	0.4648237441093741	F	F	F
0.0193452960738149	0.9848732090615910	0.6239408547374615	T	T	T
0.1625061863176891	0.3370452724513807	0.5388231950653617	T	T	T
0.3274974330528398	0.1347930324013507	0.7159636555676258	T	T	T
0.9999922729179431	0.5000441982274353	0.3790943669879780	F	F	F
0.1666222824035870	0.8333092939980062	0.2933258797492897	F	F	F
0.3333383730563639	0.6666767461127208	0.4648237441093741	F	F	F
0.9808341584066855	0.5219957540819471	0.6211763692112648	T	T	T
0.1681827890280684	0.8294513177274222	0.5338956027542978	T	T	T
0.3379716323610085	0.6638731615487254	0.6915349941067180	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6665703570940948	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468647	0.1666325478852855	0.4648237441093741	F	F	F
0.4914747990675623	0.0183015036794654	0.6185507590009839	T	T	T
0.6708826865135108	0.3319139095814517	0.5328697515439625	T	T	T
0.8471130197835429	0.1741348357879477	0.6968594758562195	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.5093613812813087	0.4655430353861610	0.6226042460649082	T	T	T
0.6636384650368560	0.8352792980385545	0.5371788846392729	T	T	T
0.8651207074211757	0.6554411447892297	0.7203718635027194	T	T	T
0.4229571979837605	0.3303705667528706	0.7408564182525825	T	T	T
0.7048438254416760	0.8051499149999528	0.7792196339682719	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1822284979606825	0.3287655105637092	0.6821364226250641	T	T	T
0.3372743629179973	0.1669079505629456	0.5608631577850701	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1712372222580412	0.8263108230231816	0.6746930372263442	T	T	T
0.3333479814155017	0.6706597219294703	0.5613888491146680	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6682140206058537	0.3304273318803663	0.6805678890364479	T	T	T
0.8273178695556745	0.1665004446534461	0.5624976604976277	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F

```
  0.6753021174177974  0.8359948678520164  0.6936732558585486   T   T   T
  0.8329145207325095  0.6643136812633209  0.5611094898758697   T   T   T
  0.6410405065658699  0.7675059915533227  0.8130048839326258   T   T   T
  0.8221305169167613  0.6858225001647311  0.7544778440060390   T   T   T
  0.3681308148520708  0.3949650736391725  0.9147002649437285   T   T   T
  0.3812615805679209  0.3953629574987946  0.8445681764908886   T   T   T
  0.1494086045124701  0.3013590239051174  0.8763716846956898   T   T   T
  0.3198912844271085  0.5588994096117949  0.8776372226922043   T   T   T
  0.3052254084924082  0.4128679724869269  0.8782809143686029   T   T   T
```

Figure S13 (b): transition state for CH_4 activation on O_2^{2-}

```
O    La   H    C
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095201    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999999
   O    La   H    C
    26    16    6    1
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093740   F   F   F
 -0.0019094047691990  0.9698892213508291  0.6224927206473707   T   T   T
  0.1655167356531530  0.3331144510320833  0.5385873943188932   T   T   T
  0.3371047417717743  0.1419346434786082  0.7019772738624204   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035880  0.8333092939980066  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093740   F   F   F
  0.9847438630086249  0.5189391702730920  0.6199073456051440   T   T   T
  0.1699347655044677  0.8324790558502289  0.5337139396979754   T   T   T
  0.3339684148063306  0.6608436748197228  0.6990353120866025   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468648  0.1666325478852855  0.4648237441093740   F   F   F
  0.4935572830021345 -0.0006258371140265  0.6176112894813534   T   T   T
  0.6657504770482071  0.3279695527225697  0.5341200938421293   T   T   T
  0.8440790010177494  0.1753340927487617  0.6944106023146802   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944196  0.8333092939980066  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093740   F   F   F
  0.5206912369561916  0.4903842653405713  0.6250112900622611   T   T   T
  0.6638877098452984  0.8344906146299612  0.5351841045760555   T   T   T
  0.8567659093099149  0.6468044254465247  0.7207184733708965   T   T   T
```

0.3519823788299865 0.2987730912961545 0.7632172061442547 T T T
0.7389806926870564 0.8339478018823531 0.7754765602744742 T T T
0.1666325478852855 0.3332650957705710 0.4388937363395371 F F F
0.3333486385380624 0.1666325478852855 0.3192558875191267 F F F
0.1804251246096463 0.3276617367459888 0.6853563171241115 T T T
0.3355029059451020 0.1629427259779523 0.5612347835149764 T T T
0.1666222824035880 0.8333092939980066 0.4388937363395371 F F F
0.3333383730563639 0.6666767461127208 0.3192558875191267 F F F
0.1665409523960142 0.8179262418975030 0.6752908989748886 T T T
0.3349146604534350 0.6702246046766782 0.5609747760885211 T T T
0.6665703570940948 0.3332650957705710 0.4388937363395371 F F F
0.8332864477468648 0.1666325478852855 0.3192558875191267 F F F
0.6690935162124170 0.3316940546246964 0.6802603558917338 T T T
0.8285362543534778 0.1638190003405628 0.5627346729067898 T T T
0.6666870115944196 0.8333092939980066 0.4388937363395371 F F F
0.8332761822651662 0.6666767461127208 0.3192558875191267 F F F
0.6720735682527081 0.8356163574837585 0.6880143172155494 T T T
0.8327302674907067 0.6654012599106615 0.5613049822666032 T T T
0.6863987049050152 0.8219886061899352 0.8103151404880089 T T T
0.8218270799277262 0.6987364689674930 0.7532487866401393 T T T
0.4532595755858341 0.4773092827305298 0.8597810145833946 T T T
0.3356357811908519 0.2997381595523372 0.8058501713114100 T T T
0.1848895321778488 0.3542258463202599 0.8508128218300161 T T T
0.3484840560633784 0.5691654637188485 0.8107692243435715 T T T
0.3305650016489969 0.4447890974635185 0.8336659239125999 T T T

Figure S13 (b): CH_3OH desorption from La_2O_3 (001) surface

O La C H
1.00000000000000
7.8789800000000003 0.0000000000000000 0.0000000000000000
-3.9394900000000002 6.8233968359095165 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5688315207999963
O La H
25 16 2
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.3790943669879780 F F F
0.1666325478852855 0.3332650957705710 0.2933258797492897 F F F
0.3333486385380624 0.1666325478852855 0.4648237441093741 F F F
0.0145097582710076 0.9845803465199702 0.6235843987504042 T T T
0.1656850328310593 0.3353707505483263 0.5383289167878269 T T T
0.3365016528653106 0.1640957257841258 0.7084441035950234 T T T
0.9999922729179431 0.5000441982274353 0.3790943669879780 F F F

0.1666222824035870	0.8333092939980062	0.2933258797492897	F	F	F
0.3333383730563639	0.6666767461127208	0.4648237441093741	F	F	F
0.9828151498846019	0.5116567064044293	0.6176670709724706	T	T	T
0.1703541099934004	0.8333056329479432	0.5337958925316167	T	T	T
0.3289013116311872	0.6588384429482480	0.6949434948275601	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6665703570940948	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468647	0.1666325478852855	0.4648237441093741	F	F	F
0.4925097270843395	0.0124481964095699	0.6202256240778119	T	T	T
0.6668787940856272	0.3301207534413294	0.5332365812356843	T	T	T
0.8415954684154743	0.1696720260441227	0.6970492120802247	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.5187011708250912	0.4866307763636817	0.6234066021461788	T	T	T
0.6636638926087328	0.8357723474848958	0.5367563086631526	T	T	T
0.8558387028933493	0.6480865087306046	0.7189544826989160	T	T	T
0.6919992861011309	0.7884235972050875	0.7757325643535751	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1743189878897176	0.3242345868430561	0.6799861049459788	T	T	T
0.3359561439061828	0.1653753909231447	0.5604482503296723	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1759674601644878	0.8393439134097456	0.6785583817414542	T	T	T
0.3321970070171182	0.6701311388843363	0.5618194984120736	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6629920084532861	0.3246864129954069	0.6789072047440926	T	T	T
0.8298214610559083	0.1684415110275999	0.5617487986353945	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6669854742005893	0.8318239047251297	0.6890346744198247	T	T	T
0.8341451479321702	0.6650391294746986	0.5617020761642536	T	T	T
0.6567646431863577	0.8001719556931955	0.8112411234671958	T	T	T
0.8126426525634478	0.6833448862077964	0.7525928804434207	T	T	T

Figure S13 (b): transition state for H transference on La_2O_3 (001) surface

```
O   La   H
  1.00000000000000
    7.8789800000000003    0.0000000000000000    0.0000000000000000
   -3.9394900000000002    6.8233968359095201    0.0000000000000000
    0.0000000000000000    0.0000000000000000   25.5688315207999999
```

```
  O   La   H
   25   16    2
Selective dynamics
Direct
 0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
 0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
 0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
 0.9962529638612051  0.9939093497843130  0.6252273847786246   T   T   T
 0.1697277506853925  0.3370751826040371  0.5376041602271341   T   T   T
 0.3290176797004226  0.1613893200313186  0.7057384512238059   T   T   T
 0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
 0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
 0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
 0.9603744309287020  0.4839827921176857  0.6184710977826666   T   T   T
 0.1707563824041788  0.8332945578616779  0.5375707588027467   T   T   T
 0.3234736513418046  0.6642404587038429  0.6856363328450655   T   T   T
 0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
 0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
 0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
 0.5187178682008196  0.0286088842878157  0.6201860262458980   T   T   T
 0.6645614765017710  0.3314381003415923  0.5314230239328114   T   T   T
 0.8364302608992633  0.1646755400691390  0.7072780958816217   T   T   T
 0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
 0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
 0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
 0.5225160270024570  0.4910344095301772  0.6203792840617303   T   T   T
 0.6618443205466352  0.8319217277976407  0.5361224088088337   T   T   T
 0.8536009811285358  0.6647460814281785  0.7148746237715756   T   T   T
 0.6091653590470588  0.6674896319532925  0.7690887459395139   T   T   T
 0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
 0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
 0.1634816904297648  0.3224541794252612  0.6818823996030590   T   T   T
 0.3407400786952455  0.1708688809521549  0.5607665582430349   T   T   T
 0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
 0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
 0.1637308284407896  0.8408525937841137  0.6772083726015355   T   T   T
 0.3351077440363865  0.6674995916654721  0.5626785368892619   T   T   T
 0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
 0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
 0.6667703359339048  0.3290630194445110  0.6805382525425235   T   T   T
 0.8297188140131857  0.1695216316975351  0.5614323985274804   T   T   T
 0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
 0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
 0.6647831424443408  0.8375113185849619  0.6835343309363479   T   T   T
```

```
  0.8286191745055573  0.6599341756854523  0.5612169647316426   T   T   T
  0.6191915307365340  0.6991878265441874  0.8059894740960043   T   T   T
  0.7513072151008470  0.6605230162091357  0.7495624994561927   T   T   T
```

Figure S13 (b): H_2O physisorption on La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   H
    25    16    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
 -0.0010187450621210  0.9950697843418169  0.6222282855968982   T   T   T
  0.1673788088742488  0.3348447191891596  0.5364497808919816   T   T   T
  0.3310760494833934  0.1663686124927863  0.7055695323042952   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
 -0.0133738298671672  0.4995537900247755  0.6189527819792359   T   T   T
  0.1687043490228529  0.8338846067658818  0.5353345335257821   T   T   T
  0.3293635701416367  0.6649714521097885  0.6991812308928151   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.5044124863636270  0.0093415096632888  0.6200083817509473   T   T   T
  0.6657835850991324  0.3321645213709748  0.5335720374769198   T   T   T
  0.8369698143708199  0.1710572145723628  0.7043388265963534   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.5100508884661596  0.4960191548746276  0.6207152866370357   T   T   T
  0.6645814028320052  0.8335734787918330  0.5352839362231281   T   T   T
  0.8404659231831441  0.6650045588284973  0.7097260443691374   T   T   T
  0.7140959439809631  0.7921227485727482  0.7852889195523568   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1666418602589002  0.3302023009902918  0.6796382413951050   T   T   T
  0.3361595574560708  0.1677306260347650  0.5608536754825756   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
```

0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1656221084520985	0.8361310551980992	0.6791847140869152	T	T	T
0.3338604524859979	0.6682771197798274	0.5613074610600954	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6667344552452956	0.3351280538758134	0.6804569839314103	T	T	T
0.8310954232391101	0.1676584314334099	0.5611881428147971	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6663489435638001	0.8376403107601154	0.6832225862947455	T	T	T
0.8319581029846372	0.6649105315787338	0.5612453062538006	T	T	T
0.8086880291803724	0.9092347483304203	0.8038483234302716	T	T	T
0.7887918901812032	0.7356055234184643	0.7669034575863246	T	T	T

Table S5 Optimized fractional coordinates for structures shown in Figure S3 & S14.

Figure S14(a): $2O_2^{2-}$ sites on La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La
    26    16
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
 -0.0078255630831968  0.0109445326211028  0.6194731047828126   T   T   T
  0.1695683633978310  0.3361053222902954  0.5350088000124196   T   T   T
  0.2982634270600202  0.1209721781866457  0.7090329968211897   T   T   T
  0.9999897345183015  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.0071724165316617  0.5064725949119965  0.6196752430695069   T   T   T
  0.1668125060567144  0.8336244718075376  0.5369399886917616   T   T   T
  0.3334098834491682  0.6703782430694607  0.6997404274999351   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.4963236342230963 -0.0026218703431821  0.6200990762402502   T   T   T
  0.6676280265484529  0.3337382236035167  0.5338595863576125   T   T   T
  0.8260843079663664  0.1771944937008900  0.7075812562088925   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.5142352626034233  0.4813324699320201  0.6239210664408793   T   T   T
  0.6646662799779239  0.8306576112916476  0.5353560741029467   T   T   T
  0.8792649639173440  0.7016075869607625  0.7079090421127373   T   T   T
  0.3728916335014817  0.2924673232683242  0.7434555181039718   T   T   T
  0.7102476440898402  0.6299661480633106  0.7431429515689285   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1561392588544647  0.3325477591663656  0.6842141158638556   T   T   T
  0.3380745216619270  0.1723391012298531  0.5611355371314001   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
```

```
  0.1793112090637834  0.8235562146922429  0.6681662770818688   T   T   T
  0.3338092761720997  0.6660985913798112  0.5594180806072888   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6513275009290018  0.3486997321957436  0.6916967907021034   T   T   T
  0.8340186934297500  0.1669227482621798  0.5629409286317358   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6710169600994945  0.8481592024078058  0.6844142983836748   T   T   T
  0.8289088856117421  0.6625566322110367  0.5610813481085781   T   T   T
```

Figure S14 (a): CH_3OH chemisorption on $2O_2^{2-}/La_2O_3$ (001) surface

```
O   La   C   H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095201    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999999
   O   La   C   H
    27   16    1    4
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0428109585475241  0.0575445695389614  0.6204424051482247   T   T   T
  0.1624346036364596  0.3355491671138456  0.5304820331245633   T   T   T
  0.3245912392584681  0.1485641081056339  0.7191463154151673   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.0139748226918542  0.4830276651578580  0.6227218123034488   T   T   T
  0.1626893003358455  0.8282381955286197  0.5397848191768282   T   T   T
  0.3235652456612698  0.6819183234404428  0.7064923873225452   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.5050321818666992  0.0194988758508080  0.6307262300716340   T   T   T
  0.6729727056847266  0.3384694019281925  0.5368493681102758   T   T   T
  0.8286390636110614  0.1704052453018846  0.7141112508717723   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.4453260424186972  0.4653825342081294  0.6173717065814353   T   T   T
```

```
  0.6686385678618645  0.8327511849772424  0.5375181800454771   T   T   T
  0.8155793978005711  0.6758024577495697  0.6637313046203495   T   T   T
  0.4335214382098788  0.3506989909277493  0.7403246081238535   T   T   T
  0.8633962227639131  0.6822384756824751  0.7203242304437020   T   T   T
  0.5784231169186932  0.7018159202032295  0.7969795605807591   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1676060768163002  0.3401124441655767  0.6816591634496140   T   T   T
  0.3302723202571559  0.1758297275716275  0.5613322514667815   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1791498314805779  0.8429556714790728  0.6737339648277162   T   T   T
  0.3317132665711958  0.6555270483889980  0.5615657874223827   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6663838915915501  0.3248550262539211  0.6835888824307416   T   T   T
  0.8409788231972815  0.1695330662718961  0.5626098242724558   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6522917833369178  0.8427661248442934  0.6991595607106789   T   T   T
  0.8312539814367396  0.6647087171781890  0.5619604769428590   T   T   T
  0.7243012414907094  0.7419756135797276  0.8363090043560514   T   T   T
  0.7997102507308580  0.9002483446841586  0.8437915667377937   T   T   T
  0.8320855784830385  0.7012347491652244  0.8230135193705060   T   T   T
  0.6555371011033186  0.6639640921245336  0.8728462826878862   T   T   T
  0.5033574990835753  0.5593700162662204  0.7905465914926708   T   T   T
```

Figure S14 (a): transition state for CH_3OH activation on $2O_2^{2-}/La_2O_3$ (001) surface

```
O   La   C   H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095201    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999999
   O   La   C   H
    27   16    1    4
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0408433072980842  0.0579474741817431  0.6219759575945428   T   T   T
  0.1629324730174073  0.3353588876961962  0.5304077468233532   T   T   T
  0.3194678135222271  0.1563321853403070  0.7241322930249054   T   T   T
```

0.9999922729179431	0.5000441982274353	0.3790943669879780	F	F	F
0.1666222824035870	0.8333092939980062	0.2933258797492897	F	F	F
0.3333383730563639	0.6666767461127208	0.4648237441093741	F	F	F
0.0147812040467270	0.4791373916780631	0.6201869103217199	T	T	T
0.1617456562043211	0.8301690014505203	0.5381634313848523	T	T	T
0.3220917874272070	0.6867951141836295	0.7061306131366957	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6665703570940948	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468647	0.1666325478852855	0.4648237441093741	F	F	F
0.4896009075074815	0.0245409455556003	0.6312930758612707	T	T	T
0.6706640333212999	0.3387798583879253	0.5369405541213508	T	T	T
0.8190314934156329	0.1679306859874665	0.7111650840602460	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.4415709587137129	0.4680077537121966	0.6197885917522608	T	T	T
0.6666089357709727	0.8340795853652189	0.5397851843787167	T	T	T
0.8231458743098672	0.6722887799158087	0.6615994285304548	T	T	T
0.4325037355354907	0.3621158506094441	0.7424115051088070	T	T	T
0.8485125481364645	0.7103925541954110	0.7364113441940210	T	T	T
0.5500481480920559	0.6657087978050715	0.8048800637138960	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1619384288972834	0.3432839404070232	0.6816428846986984	T	T	T
0.3292389981910873	0.1740853157086970	0.5620483558900320	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1684963063019096	0.8487823860509095	0.6800168313707279	T	T	T
0.3256077341178916	0.6556022417566442	0.5616730866293700	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6591812455203171	0.3295933755242385	0.6841040744761452	T	T	T
0.8422625034179244	0.1744911856678910	0.5619511248652402	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6492964186231106	0.8421314761173522	0.6880607303788243	T	T	T
0.8324080910559302	0.6662333604640925	0.5627047339068849	T	T	T
0.7301374360748345	0.7134872144451579	0.8231419899146246	T	T	T
0.8065153343957308	0.8621798586300745	0.8393923439078376	T	T	T
0.8354360162522216	0.7254532747115313	0.7825229925547932	T	T	T
0.7410040188139292	0.6010745579506644	0.8459900379499780	T	T	T
0.4798312547519377	0.5269758244458606	0.7911442227814877	T	T	T

Figure S14 (a): $CH_2(OH)_2$ physisorption on O_2^{2-}/La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   C    H
    27    16    1    4
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0158832138235970  0.0008179432192956  0.6240677727244985   T   T   T
  0.1643209438601052  0.3383000609793794  0.5375631664366641   T   T   T
  0.3197497162931590  0.1423265425442905  0.7162834159715371   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
 -0.0196031558923440  0.5023082084763485  0.6213580807566509   T   T   T
  0.1661069363772835  0.8283811047149101  0.5356763451909247   T   T   T
  0.3353620013546288  0.6676259410147857  0.6896127252595113   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.4983539710485013  0.0276102376368815  0.6182121641808158   T   T   T
  0.6711523757119812  0.3345178583373643  0.5321597654428681   T   T   T
  0.8358971348951639  0.1662944871071063  0.7040089508815384   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.5100729224251327  0.4723514867754314  0.6202896179023012   T   T   T
  0.6640642910652189  0.8336028993327208  0.5367355481800370   T   T   T
  0.8522148567528300  0.6690862474056236  0.7105319820055550   T   T   T
  0.4162530675635225  0.3425438428266084  0.7386440809121217   T   T   T
  0.8661895877846473  0.8474202152468234  0.7983763290964946   T   T   T
  0.5250860334393710  0.6814309305136914  0.7922360520076153   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1648014327453994  0.3265055275265845  0.6794451312282703   T   T   T
  0.3387287944932576  0.1692503202972903  0.5608328554822888   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1631113116178544  0.8277950206063308  0.6747293624261872   T   T   T
  0.3343247484868030  0.6691320007689104  0.5619535996618645   T   T   T
```

```
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6685758151849739  0.3371050138449191  0.6808533013394635   T   T   T
  0.8278632617411724  0.1672642983465142  0.5619267345735232   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6727171225928426  0.8311306976242923  0.6939006395313740   T   T   T
  0.8296522990226197  0.6621036830877343  0.5609101366281353   T   T   T
  0.6913215677161031  0.7376085571614726  0.8262089745350428   T   T   T
  0.6868441189672743  0.8333140578723124  0.8567553197629879   T   T   T
  0.8748779640382834  0.7596408350596403  0.7709201987211031   T   T   T
  0.6797245214845515  0.6042312443360909  0.8438159777313216   T   T   T
  0.4598984652828841  0.5390761027808850  0.7855771958064173   T   T   T
```

Figure S14 (a): transition state for $CH_2(OH)_2$ dissociation with H_2O

```
C   H   O
   1.00000000000000
    14.5000000000000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.0000000000000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.5000000000000000
   C   H   O
     1    6    3
Selective dynamics
Direct
  0.5014992414802543  0.5087841799596273  0.5096079984155797   T   T   T
  0.4894858302785715  0.5751035336299926  0.5393088000686116   T   T   T
  0.4997817827519857  0.4529304086856667  0.5557118889212732   T   T   T
  0.3454389087017373  0.5286740521924472  0.4991781904559692   T   T   T
  0.5215232318969267  0.5517788892190271  0.3869161428050062   T   T   T
  0.4088258238546196  0.5404911288231677  0.4020731464172260   T   T   T
  0.4561643536438492  0.5622638431833917  0.2918896684075982   T   T   T
  0.5587728204566368  0.5031150450490436  0.4460361580290567   T   T   T
  0.3897226376039458  0.4965390833933463  0.4633727854840426   T   T   T
  0.4593337669442557  0.5841838254027550  0.3508264123348998   T   T   T
```

Figure S14 (a): CH_2O chemisorption on O_2^{2-}/La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O   La   C   H
    26   16    1    2
Selective dynamics
```

Direct

0.0000000000000000	0.0000000000000000	0.3790943669879780	F	F	F
0.1666325478852855	0.3332650957705710	0.2933258797492897	F	F	F
0.3333486385380624	0.1666325478852855	0.4648237441093741	F	F	F
0.0135160603497339	0.0069432066321862	0.6199681927634740	T	T	T
0.1642327898209312	0.3356468886306282	0.5347828604629424	T	T	T
0.3187099557932767	0.1378445977335771	0.7142513439092096	T	T	T
0.9999922729179431	0.5000441982274353	0.3790943669879780	F	F	F
0.1666222824035870	0.8333092939980062	0.2933258797492897	F	F	F
0.3333383730563639	0.6666767461127208	0.4648237441093741	F	F	F
0.0025664312921755	0.5085164308984149	0.6209464951801040	T	T	T
0.1644948073139343	0.8290938397354825	0.5347137655734223	T	T	T
0.3318137629896656	0.6709542610870520	0.7016757419388115	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6665703570940948	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468647	0.1666325478852855	0.4648237441093741	F	F	F
0.4943739294863712	0.0083730215859390	0.6195767531921814	T	T	T
0.6709916545032573	0.3353900996572358	0.5344415622239551	T	T	T
0.8370678856921802	0.1737918895381678	0.7031276797965452	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.4876826247618309	0.4729358607815157	0.6212440680949199	T	T	T
0.6659340200940305	0.8324346008514599	0.5361597364744293	T	T	T
0.8388292509312402	0.6714611292771802	0.7027026180752182	T	T	T
0.4146701822674465	0.3307807645514724	0.7406358547776530	T	T	T
0.6512737228918439	0.8217001676531488	0.7938433415996667	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1717060088621482	0.3372542339517194	0.6810876359349001	T	T	T
0.3339076167022091	0.1675246948477952	0.5610895025924757	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1603854560485233	0.8224510389693998	0.6753567983343516	T	T	T
0.3325078542782293	0.6663385992780181	0.5607494434608949	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6656119112455141	0.3379595783795324	0.6813180994050321	T	T	T
0.8325143479428251	0.1661837232291584	0.5620096430582636	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6688387995576424	0.8377445388293964	0.6874551602113715	T	T	T
0.8330815157317957	0.6657420329922744	0.5607152068129210	T	T	T
0.5764739773897800	0.6731822468509103	0.8207168779137983	T	T	T

```
  0.5714703682117157  0.6852256073105364  0.8639957137093270   T   T   T
  0.5117524725420980  0.5241890464824536  0.8033400623407705   T   T   T
```

Figure S14 (b): transition state for CH_2O activation on O_2^{2-}/La_2O_3 (001) surface

```
O    La   C    H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095201    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999999
   O    La   C    H
    26    16    1    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093740   F   F   F
 -0.0034419959456976  0.0051926881471912  0.6200106962925132   T   T   T
  0.1677539803267665  0.3347013920188426  0.5344687734148533   T   T   T
  0.3224298699323683  0.1446457524877772  0.7041825185794002   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035880  0.8333092939980066  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093740   F   F   F
  1.0043815638407179  0.5018598273973641  0.6212494732565351   T   T   T
  0.1663897035914429  0.8324479652306144  0.5364184611143951   T   T   T
  0.3351663111390910  0.6740143047473348  0.7032518472708901   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468648  0.1666325478852855  0.4648237441093740   F   F   F
  0.5096341578314961  0.0070801937053367  0.6202870771830594   T   T   T
  0.6680039351979701  0.3354136081656381  0.5347933079488133   T   T   T
  0.8403183926873649  0.1767919131623949  0.7067916536577896   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944196  0.8333092939980066  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093740   F   F   F
  0.4934846933950057  0.4880600108448751  0.6208722540537606   T   T   T
  0.6661362654118499  0.8317187381109694  0.5348577676195835   T   T   T
  0.8418153583401519  0.6734894297732743  0.7025227635846509   T   T   T
  0.4439981795558738  0.3619582319106728  0.7542159112448298   T   T   T
  0.6151448682039805  0.7705561123929077  0.7965297293057215   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1756328928974414  0.3415489457566003  0.6838673285099325   T   T   T
  0.3351274341516322  0.1698831887910896  0.5613183312703530   T   T   T
```

```
  0.1666222824035880  0.8333092939980066  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1628340416334003  0.8219501031883153  0.6753798620744296   T   T   T
  0.3345864532691643  0.6651294526033772  0.5609211702698192   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468648  0.1666325478852855  0.3192558875191267   F   F   F
  0.6676133904893299  0.3380575646526740  0.6827224320736082   T   T   T
  0.8338340988424262  0.1662957865552868  0.5621668930051043   T   T   T
  0.6666870115944196  0.8333092939980066  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6750413976323413  0.8441554708185036  0.6837411972910787   T   T   T
  0.8315697303385634  0.6663244359782080  0.5608861928007348   T   T   T
  0.5279043587733420  0.6014800428695405  0.8087964035751104   T   T   T
  0.4259550835864642  0.5373576418971057  0.8424503578032941   T   T   T
  0.5498985979330921  0.4624881221435969  0.7849403168445833   T   T   T
```

Figure S14 (b): HCOOH chemisorption on La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   C    H
    26    16    1    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0095235750220442  0.0084281124135406  0.6215474121298492   T   T   T
  0.1663170256564671  0.3339326638512477  0.5342719458772547   T   T   T
  0.3331753246999538  0.1665684446762222  0.7085824949250333   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.9954920856225983  0.4918071702345633  0.6181944617541981   T   T   T
  0.1654233433778304  0.8312232639580381  0.5354118211110216   T   T   T
  0.3290865843743349  0.6656860257832194  0.7026083595028155   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.4984973108799675  0.0096141990338826  0.6213851273370868   T   T   T
  0.6673074667631876  0.3341569072462419  0.5342950617847757   T   T   T
  0.8334297458177460  0.1671615032780812  0.7059902467151153   T   T   T
```

```
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.4933110789607575  0.4880801765212554  0.6203750688061187   T   T   T
  0.6657682321756226  0.8319870188663918  0.5359765696610480   T   T   T
  0.8362670691210187  0.6652599839608855  0.7026213096319556   T   T   T
  0.6374585733945077  0.7764477571298321  0.7923904111527748   T   T   T
  0.5904108942782980  0.6592902831366790  0.8753745590934856   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1659894153873296  0.3300351892520659  0.6799250122054032   T   T   T
  0.3335963614562212  0.1674672369991183  0.5607827663621738   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1690362826846486  0.8387748609026934  0.6795220595350986   T   T   T
  0.3315494947815174  0.6641896526063872  0.5614154519339714   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6636199116915792  0.3296820831070761  0.6797490402593082   T   T   T
  0.8337099598878212  0.1680756313569529  0.5613183194024036   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6663960219767978  0.8328065908016686  0.6854348186753837   T   T   T
  0.8323707415746872  0.6644432896946008  0.5614129143988651   T   T   T
  0.6398529188101424  0.8012223711110511  0.8393614998108317   T   T   T
  0.6823915300698993  0.9422279540202844  0.8586787546323900   T   T   T
  0.5541305938591558  0.5371661285077038  0.8564416517036449   T   T   T
```

Figure S14 (c): HCOOH chemisorption on $2O_2^{2-}/La_2O_3$ (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   C    H
    28    16    1    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
 -0.0007421798960098  0.0011979914964308  0.6210214181639293   T   T   T
  0.1679152084864114  0.3380693375740080  0.5360323799283784   T   T   T
  0.2968614689374054  0.1139935173184070  0.7138377004320584   T   T   T
```

0.9999922729179431	0.5000441982274353	0.3790943669879780	F	F	F
0.1666222824035870	0.8333092939980062	0.2933258797492897	F	F	F
0.3333383730563639	0.6666767461127208	0.4648237441093741	F	F	F
0.9850067723176722	0.5009859398931752	0.6198142509369713	T	T	T
0.1681535967075845	0.8314720402255467	0.5366544162827243	T	T	T
0.3389744308787678	0.6664989179303725	0.6884345923856018	T	T	T
0.4999378092088094	0.0000000000000000	0.3790943669879780	F	F	F
0.6665703570940948	0.3332650957705710	0.2933258797492897	F	F	F
0.8332864477468647	0.1666325478852855	0.4648237441093741	F	F	F
0.4938598522009160	0.0196366307168931	0.6192814225925051	T	T	T
0.6684023108493461	0.3323214701477800	0.5321193273918200	T	T	T
0.8207785315802568	0.1636745343046964	0.7034800519636586	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.5282387759274614	0.4795775050367186	0.6230598978963574	T	T	T
0.6620886687822809	0.8321708900118525	0.5373138459625895	T	T	T
0.8828171455978895	0.6958213442751700	0.7102354112621406	T	T	T
0.7050797896582625	0.6249469429425033	0.7416826057761906	T	T	T
0.1075303200577006	0.4148921284604037	0.7862677292168309	T	T	T
0.3876601408726424	0.2865069535879423	0.7478175347027149	T	T	T
0.2611882768941081	0.2982815736749395	0.8379815443413079	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1545439388730425	0.3300361496017012	0.6899666749879986	T	T	T
0.3398243701641395	0.1723171895743289	0.5611755875630154	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1756875882165885	0.8263730294753587	0.6674699920563404	T	T	T
0.3319036121897537	0.6657252145558841	0.5603717196190418	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6580198598950070	0.3432330903281989	0.6878432911682381	T	T	T
0.8329984537952329	0.1706748646553479	0.5632087241339158	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6776094776207551	0.8388327780027136	0.6804885612260255	T	T	T
0.8287545784653240	0.6596168112201295	0.5606066423081523	T	T	T
0.1552336359002946	0.3814231922319352	0.8295674545709778	T	T	T
0.1089522196667944	0.4214536935665197	0.8661118274432247	T	T	T
0.3093417245232338	0.2733893083616086	0.8018797340500096	T	T	T

Figure S14 (c): transition state for HCOOH activation on $2O_2^{2-}/La_2O_3$ (001) surface

```
O   La   C   H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095201    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999999
   O   La   C   H
    28   16    1    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0128864178356760  0.0029190498833045  0.6216499973004360   T   T   T
  0.1637846019459719  0.3377182755020837  0.5364126686992491   T   T   T
  0.3054314712556898  0.1273807875874914  0.7169984690636380   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.9844118511397292  0.5058152447617038  0.6202585099609348   T   T   T
  0.1661521677480862  0.8288516169060055  0.5353144388772626   T   T   T
  0.3328792535887585  0.6663491968154537  0.6925051682994718   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.4934386152545523  0.0245671046866434  0.6207350762858995   T   T   T
  0.6699026827293079  0.3334818955418205  0.5326789357687368   T   T   T
  0.8371784622287158  0.1725799213188798  0.7021110134372308   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.5022216459078980  0.4685129655489556  0.6213626959958126   T   T   T
  0.6627971609310286  0.8331314149983399  0.5376998996224356   T   T   T
  0.8528513278518824  0.6734463535745145  0.7067712919235365   T   T   T
  0.7030589121872023  0.6856371693427202  0.7596696341048216   T   T   T
  0.4338153608913197  0.7932244779006106  0.8371959557931232   T   T   T
  0.4092814819704277  0.3243939917585234  0.7407159752674898   T   T   T
  0.3191629885111015  0.4719117648182747  0.8189224358683282   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1662111589083475  0.3296732347436263  0.6807057456109737   T   T   T
  0.3363958028480659  0.1690248817325433  0.5609831150719031   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1690239947391064  0.8277174662335915  0.6742779702482641   T   T   T
```

```
  0.3309067864596006  0.6663828495783168  0.5608215575006464   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6606840177546204  0.3309673163050876  0.6832962649708909   T   T   T
  0.8303548770710594  0.1688730477182697  0.5618999108770382   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6741968342685121  0.8368335404976044  0.6846788880709256   T   T   T
  0.8308916403983120  0.6615255523250583  0.5608903648555297   T   T   T
  0.4499114472362883  0.6606240034747058  0.8192078426532179   T   T   T
  0.6050663654367633  0.6931360795567639  0.7986080456675987   T   T   T
  0.3625508233339676  0.3970149819581469  0.7947540845522680   T   T   T
```

Figure S14 (c): $CO(OH)_2$ physisorption on O_2^{2-}/La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   C    H
    28    16    1    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0146019001662878 -0.0015854535673438  0.6231206794248220   T   T   T
  0.1651371102095461  0.3367484474351075  0.5371197159145156   T   T   T
  0.3199938121227651  0.1423253409220325  0.7167918991204444   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.9886812693607219  0.5048715614706031  0.6215509404453086   T   T   T
  0.1663198235548151  0.8287368455594400  0.5350064919128570   T   T   T
  0.3351252823594108  0.6674524700340665  0.6935841351236152   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.5001841461481559  0.0196929539425151  0.6188610905624573   T   T   T
  0.6713533489657081  0.3344413914362784  0.5330478016841808   T   T   T
  0.8402485521344351  0.1692613497383279  0.7021655658790366   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
```

```
  0.5021554285724450  0.4708019337304278  0.6212448833615258   T   T   T
  0.6653349545990170  0.8326164785020348  0.5372272026812592   T   T   T
  0.8404829752300784  0.6692519348142828  0.7069198503958352   T   T   T
  0.6082557720163491  0.7311830183652118  0.7884289305553015   T   T   T
  0.3752543774707636  0.7934066652057506  0.8176194927238178   T   T   T
  0.4184325936077204  0.3389496252113514  0.7409230673488082   T   T   T
  0.3109515805882285  0.4796248377893198  0.8176683917300585   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1693724754112757  0.3320525619242185  0.6792135107941611   T   T   T
  0.3375955336708932  0.1669397898206459  0.5613463673956075   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1588120472693910  0.8228990514313531  0.6788000083485295   T   T   T
  0.3330680264239385  0.6686228212487028  0.5614740841077714   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6697159003938039  0.3367476988865278  0.6814196550893583   T   T   T
  0.8299645049377454  0.1674608798616828  0.5615404572369637   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6751002424899508  0.8360570291793215  0.6853579880087115   T   T   T
  0.8330644595611247  0.6631468553237195  0.5609761043263619   T   T   T
  0.4225463607897680  0.6718697281928591  0.8090201831930272   T   T   T
  0.6400029507776072  0.6254833502084972  0.7876951463785496   T   T   T
  0.3510271356518533  0.3999010806389777  0.7947415433361209   T   T   T
```

Figure S14 (c): transition state for $CO(OH)_2$ dissociation with H_2O

```
C   O   H
   1.00000000000000
    14.5000000000000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.0000000000000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.5000000000000000
   C   O   H
     1    4    4
Selective dynamics
Direct
  0.4674700474890626  0.5160400090102736  0.4998177198187060   T   T   T
  0.4201290441993132  0.6135066911743614  0.5117345198567751   T   T   T
  0.5503113842509588  0.5183435967347149  0.5044245676930447   T   T   T
  0.4040764093504243  0.4601911058931683  0.4891608106775280   T   T   T
  0.2771056291168739  0.5613358804165373  0.4580467831975956   T   T   T
  0.3219783265888441  0.5031654234558125  0.4709470643823938   T   T   T
  0.4642299512773923  0.6578345044950283  0.4915102479938172   T   T   T
```

```
  0.2262101721689945  0.5621675934978128  0.4990053164003282   T   T   T
  0.3404724261499322  0.6051816874614926  0.4822513951443759   T   T   T
```

Figure S14 (c): CO_2 and H_2O physisorption on O_2^{2-}/La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La   C    H
   28    16    1    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0145444663413833  0.0098015463142420  0.6197608224132630   T   T   T
  0.1645209933895066  0.3355954259749561  0.5345665236478333   T   T   T
  0.3213033089960451  0.1394288732703657  0.7143539752214402   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.0056159897634948  0.5092348720445826  0.6215546383150080   T   T   T
  0.1647496696428787  0.8296958534295217  0.5350029521082863   T   T   T
  0.3327184196212806  0.6727861032166965  0.7030278913969004   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.4949812625853459  0.0058720759829179  0.6202423166248495   T   T   T
  0.6713336565860778  0.3359113094008001  0.5351875863929049   T   T   T
  0.8366513940829771  0.1732972674721476  0.7029788729355481   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.4846458885066946  0.4743362425215430  0.6214603690738754   T   T   T
  0.6666535435645229  0.8325731264652121  0.5363771791565628   T   T   T
  0.8380619542709928  0.6735426022583049  0.7010944067121578   T   T   T
  0.5033084110627092  0.4361813472887856  0.8447691348382665   T   T   T
  0.6124962304596354  0.8370300811544944  0.7974232632816376   T   T   T
  0.4196487746969160  0.3328759304582803  0.7403365154722978   T   T   T
  0.3001074905447050  0.6817484473953760  0.8363319420818845   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
```

```
  0.1725250032498145  0.3390005599670263  0.6819328855608205   T   T   T
  0.3334091091482957  0.1680615525638142  0.5611157885760804   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1615067212529575  0.8234981338558536  0.6756602407235222   T   T   T
  0.3327809218474793  0.6660654936744419  0.5607211221912451   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6678503781961810  0.3391532541423372  0.6807494556107963   T   T   T
  0.8338501441257601  0.1662947344934311  0.5619152371610101   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6682939986252472  0.8388721997694086  0.6864322901937825   T   T   T
  0.8340752606783438  0.6667775881515737  0.5606729706725985   T   T   T
  0.4554744178946229  0.7541453533501755  0.8170230633843920   T   T   T
  0.6409581184348738  0.4768448140620068  0.8492175225576428   T   T   T
  0.4682073038544132  0.3747629486532353  0.8097689909915244   T   T   T
```

Figure S14 (c): O_2^{2-}/La_2O_3 (001) surface

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La
    25    16
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0048913375830531  0.0064161602522522  0.6191503584645116   T   T   T
  0.1645981308078525  0.3349508308681150  0.5344538945980912   T   T   T
  0.3181380052495491  0.1389125771255949  0.7120492725038753   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.0051062315410948  0.5076599089197228  0.6224463767588246   T   T   T
  0.1645959307435986  0.8304129995681945  0.5353897280658153   T   T   T
  0.3343782439748086  0.6750974648986789  0.7035739746893565   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.4982885363711962  0.0020719188467995  0.6200846212926984   T   T   T
```

0.6695087070070150	0.3353922416723167	0.5351801514419777	T	T	T
0.8333125882566612	0.1705119416271016	0.7052572998604003	T	T	T
0.5000544637091338	0.5000441982274353	0.3790943669879780	F	F	F
0.6666870115944192	0.8333092939980062	0.2933258797492897	F	F	F
0.8332761822651662	0.6666767461127208	0.4648237441093741	F	F	F
0.4856101879400539	0.4796341073136178	0.6210590301565414	T	T	T
0.6660137521577545	0.8321396422250652	0.5357429737850973	T	T	T
0.8367947856489283	0.6746523810164335	0.7017835004166153	T	T	T
0.4134497426777075	0.3284724841399335	0.7399755105759891	T	T	T
0.1666325478852855	0.3332650957705710	0.4388937363395371	F	F	F
0.3333486385380624	0.1666325478852855	0.3192558875191267	F	F	F
0.1708677164552190	0.3404934439187255	0.6830645557300210	T	T	T
0.3329817989769532	0.1686463906179326	0.5613306603044218	T	T	T
0.1666222824035870	0.8333092939980062	0.4388937363395371	F	F	F
0.3333383730563639	0.6666767461127208	0.3192558875191267	F	F	F
0.1598019071367357	0.8209941324304969	0.6758387413883014	T	T	T
0.3327873148313606	0.6656608070850439	0.5606385918431470	T	T	T
0.6665703570940948	0.3332650957705710	0.4388937363395371	F	F	F
0.8332864477468647	0.1666325478852855	0.3192558875191267	F	F	F
0.6662242019542689	0.3396040568437361	0.6829271109843615	T	T	T
0.8332133523236127	0.1659904849894689	0.5619126702021007	T	T	T
0.6666870115944192	0.8333092939980062	0.4388937363395371	F	F	F
0.8332761822651662	0.6666767461127208	0.3192558875191267	F	F	F
0.6666609639764934	0.8395598190611778	0.6828397773318085	T	T	T
0.8328165701030464	0.6666873085569034	0.5607064655887046	T	T	T

Table S6. INCAR for structural optimization.

```
ENCUT = 520.000000
BMIX = 0.000010
AMIX_MAG = 0.800000
BMIX_MAG = 0.000010
AMIX = 0.200000
EDIFF = 1.00e-05
EDIFFG = -2.00e-02
SIGMA = 0.050000
PREC = Accurate
ISMEAR = 0
NELMIN = 6
ISPIN = 2
LORBIT = 11
NSW = 600
IBRION = 2
ISIF = 0
LCHARG = .FALSE.
LWAVE = .FALSE.
```

Table S7. INCAR for frequency analysis.

```
INCAR created by Atomic Simulation Environment
ENCUT = 520.000000
BMIX = 0.000010
AMIX_MAG = 0.800000
BMIX_MAG = 0.000010
AMIX = 0.200000
SIGMA = 0.050000
EDIFF = 1e-8
PREC = Accurate
ISMEAR = 0
NELMIN = 6
LORBIT = 11
NSW = 200
ISPIN=2
IBRION = 5
ISIF = 0
LCHARG = .FALSE.
LWAVE = .FALSE.
NFREE = 2
```

Table S8. INCAR for transition search with the dimer method.

```
LCHARG=.FALSE.
LWAVE=.FALSE.
PREC=Accurate
ENCUT=520
BMIX = 0.000010
AMIX_MAG = 0.800000
BMIX_MAG = 0.000010
AMIX = 0.200000
NELMIN=6
NSW=600
ISPIN=2
IBRION=3
ISIF=0
EDIFFG=-5.00e-02
LORBIT    = 11
ISMEAR=0
SIGMA=0.05
POTIM=0.0
ICHAIN=2
IOPT = 2
EDIFF    = 1E-7
DdR    = 5E-3
DRotMax      = 4
DFNMax       = 1.0
DFNMin       = 0.01
```

Table S9. KPOINTS value throughout the calculations over the La_2O_3 (001) surface.

```
KPOINTS created by Atomic Simulation Environment
0
Gamma
3 3 1
0 0 0
```