Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

First-Principles-Based Kinetic Monte Carlo Simulations of CO oxidation on catalytic Au(110) and Ag(110) surfaces

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INCAR file used for the geometry optimization of CO on Ag(110) through DFT calculations:

```
Test Ag(110)
Start parameters for this run

NWRITE =      2
ISTART =      0
GGA    =     91
PREC   =    high
ENCUT = 415.0

Electronic Relaxation
EDIFF  = 0.1E-06
EDIFFG = -0.001
LREAL  = Auto

Ionic relaxation
IBRION =   2
ISIF   =   2
NSW    =  400
POTIM  =   0.05
ISPIN  =   2

Electronic relaxation 2 (details)
ALGO   =  FAST


 DOS related values:
   ISMEAR =     0 ; SIGMA = 0.01
   EMIN   =   -15 ;  EMAX = 0

 Write flags
   LWAVE  =      F    do not write WAVECAR
   LCHARG =      F    do not write CHGCAR
```

POSCAR (CONTCAR) file used for the geometry optimization of CO on Ag(110) through DFT calculations:

```
Ag(110)
  1.00744422890398
    5.8322200000000004    0.0000000000000000    0.0000000000000000
    0.0000000000000000    8.2479999999999993    0.0000000000000000
    0.0000000000000000    0.0000000000000000   20.0000000000999982
  C    O    Ag
    1    1    16
Selective dynamics
Direct
  0.4962386221030325  0.7507326511565935  0.3016874420923117   T   T   T
  0.4955925759446806  0.7516115935239577  0.3592762869572122   T   T   T
  0.7517251443952352  0.7500072619527761  0.2173090337374005   T   T   T
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.4999811392574358  0.0000000000000000  0.0000000000000000   F   F   F
  0.0000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.4999811392574358  0.5000000000000000  0.0000000000000000   F   F   F
  0.2499905696287144  0.2500000000000000  0.0728999999996347   F   F   F
  0.7499717088861502  0.2500000000000000  0.0728999999996347   F   F   F
  0.2499905696287144  0.7500000000000000  0.0728999999996347   F   F   F
  0.7499717088861502  0.7500000000000000  0.0728999999996347   F   F   F
 -0.0004999207962698 -0.0022824485014823 0.1493404586470423   T   T   T
  0.4996236164400201  0.0012720687248133  0.1461611198243354   T   T   T
 -0.0004949040425780  0.5023375743687787  0.1493358270841700   T   T   T
  0.4996294552940754  0.4987725602537054  0.1461496111238449   T   T   T
  0.2485440905636731  0.2500573365230593  0.2139299736590298   T   T   T
  0.7504594685959893  0.2500555177081815  0.2139675662608982   T   T   T
  0.2455278922712394  0.7500118319883584  0.2170259553709728   T   T   T
```

POSCAR (CONTCAR) file used for the geometry optimization of O_2 on Ag(110) through DFT calculations:

```
Ag(110)
   1.007444228903977
    5.8322200000000000    0.0000000000000000    0.0000000000000000
    0.0000000000000000    8.2479999999999990    0.0000000000000000
    0.0000000000000000    0.0000000000000000   20.0000000001000000
  O Ag
  2  16
Selective dynamics
Direct
  0.3728566589046079  0.4996492356895919  0.2708012579892363   T   T   T
  0.6205924473114957  0.4996362738951442  0.2707739538571619   T   T   T
  0.7503791933151681  0.7347248293629201  0.2163233057211892   T   T   T
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.4999811392574358  0.0000000000000000  0.0000000000000000   F   F   F
  0.0000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.4999811392574358  0.5000000000000000  0.0000000000000000   F   F   F
  0.2499905696287144  0.2500000000000000  0.0728999999996347   F   F   F
  0.7499717088861502  0.2500000000000000  0.0728999999996347   F   F   F
  0.2499905696287144  0.7500000000000000  0.0728999999996347   F   F   F
  0.7499717088861502  0.7500000000000000  0.0728999999996347   F   F   F
  0.9994094059659201  0.9997821804965286  0.1566170287898145   T   T   T
  0.4995100834321814  0.9998832718213897  0.1531803822103046   T   T   T
  0.9994537089150642  0.4999634114783213  0.1408026174531850   T   T   T
  0.4996106735609010  0.4999400734476789  0.1385244449248386   T   T   T
  0.2470349915720008  0.2645651758309730  0.2162102854233024   T   T   T
  0.7504165370213682  0.2647788353793024  0.2162746712925508   T   T   T
  0.2471544043867646  0.7351102421816766  0.2162846160010979   T   T   T
```

INCAR file used to run DIMER calculations:

```
Optimization
Start parameters for this run

ISTART =   0
ISPIN  =     2
GGA    =    91

# Electronic Relaxation
ENCUT  = 415.0
IBRION=3
EDIFF  = 1E-06
EDIFFG=-0.001
POTIM=0.0
ISYM=0
NSW=900
PREC=High
LREAL=.FALSE.
LWAVE=.FALSE.
LCHARG=.FALSE.

# DIMER PARAMETERS
ICHAIN=2
DdR=0.005
DRotMax=4
DFNMin=0.01
DFNMax=1.0

# OPTIMIZER PARAMETERS
IOPT=2
```

POSCAR (CONTCAR) file used for the search of the TS structure for the O_2 dissociation:

```
Ag110
  1.00744422890398
    5.8322200000000004    0.0000000000000000    0.0000000000000000
    0.0000000000000000    8.2479999999999993    0.0000000000000000
    0.0000000000000000    0.0000000000000000   20.0000000000999982
  O    Ag
    2    16
Selective dynamics
Direct
  0.4999701584191386  0.4134881524424994  0.2442110260855010  T  T  T
  0.4999643758119373  0.6380929416662361  0.2768671901171664  T  T  T
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.4999811392574358  0.0000000000000000  0.0000000000000000  F  F  F
  0.0000000000000000  0.5000000000000000  0.0000000000000000  F  F  F
  0.4999811392574358  0.5000000000000000  0.0000000000000000  F  F  F
  0.2499905696287143  0.2500000000000000  0.0728999999996347  F  F  F
  0.7499717088861502  0.2500000000000000  0.0728999999996347  F  F  F
  0.2499905696287143  0.7500000000000000  0.0728999999996347  F  F  F
  0.7499717088861502  0.7500000000000000  0.0728999999996347  F  F  F
  0.9999740377161110  0.9952103048046119  0.1493958635840936  T  T  T
  0.4999772568031318  0.9989049247552454  0.1477407928791213  T  T  T
  0.9999788610247544  0.5002064844099162  0.1441152022467704  T  T  T
  0.4999784330751861  0.5062449197550146  0.1403396216060653  T  T  T
  0.2376828033658569  0.2426412393176277  0.2157725793188580  T  T  T
  0.7622673326367826  0.2426437013244918  0.2157725123269411  T  T  T
  0.2405863834658549  0.7503799846586369  0.2183793328862484  T  T  T
  0.7593530344673876  0.7503771069183887  0.2183798090370821  T  T  T
```

To run the kMC simulations using the kmos code please see the GitHub site: https://github.com/mhoffman/kmos