Enhanced Mass Transfer in the Step Edge Induced Oxidation on Cu (100) Surface

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Reactive force field: Cu/O/H force field; Zhu et al., J. Phys. Chem. Lett. 2016, 7, 2530-2536; Zhu et al., J. Phys. Chem. C 2017

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 39           ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.5469 !Overcoordination parameter
   26.5405 !Valency angle conjugation parameter
    1.7224 !Triple bond stabilisation parameter
    6.8702 !Triple bond stabilisation parameter
   60.4850 !C2-correction
    1.0588 !Undercoordination parameter
    4.6000 !Triple bond stabilisation parameter
   12.1176 !Undercoordination parameter
   13.3056 !Undercoordination parameter
  -70.5044 !Triple bond stabilization energy
    0.0000 !Lower Taper-radius
   10.0000 !Upper Taper-radius
    2.8793 !Not used
   33.8667 !Valency undercoordination
    6.0891 !Valency angle/lone pair parameter
    1.0563 !Valency angle
    2.0384 !Valency angle parameter
    6.1431 !Not used
    6.9290 !Double bond/angle parameter
    0.3989 !Double bond/angle parameter: overcoord
    3.9954 !Double bond/angle parameter: overcoord
   -2.4837 !Not used
    5.7796 !Torsion/BO parameter
   10.0000 !Torsion overcoordination
    1.9487 !Torsion overcoordination
   -1.2327 !Conjugation 0 (not used)
    2.1645 !Conjugation
    1.5591 !vdWaals shielding
    0.1000 !Cutoff for bond order (*100)
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    2.1365 !Valency angle conjugation parameter
    0.6991 !Overcoordination parameter
   50.0000 !Overcoordination parameter
    1.8512 !Valency/lone pair parameter
    0.5000 !Not used
   20.0000 !Not used
    5.0000 !Molecular energy (not used)
    0.0000 !Molecular energy (not used)
    2.6962 !Valency angle conjugation parameter
 5       ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
                alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
                cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
                ov/un;val1;n.u.;val3,vval4
H       0.8930    1.0000    1.0080    1.3550    0.0930    0.8203   -0.1000    1.0000
        8.2230   33.2894    1.0000    0.0000  121.1250    3.7248    9.6093    1.0000
       -0.1000    0.0000   55.6606    3.0408    2.4197    0.0003    1.0698    0.0000
      -19.4571    4.2733    1.0338    1.0000    2.8793    0.0000    0.0000    0.0000
O       1.2450    2.0000   15.9990    2.3890    0.1000    1.0898    1.0548    6.0000
        9.7300   13.8449    4.0000   37.5000  116.0768    8.5000    8.3122    2.0000
        0.9049    0.4056   63.0626    3.5027    0.7640    0.0021    0.9745    0.0000
       -3.5500    2.9000    1.0493    4.0000    2.9225    0.0000    0.0000    0.0000
Cu      1.9202    2.0000   63.5460    1.9221    0.2826    1.0000    0.1000    1.0000
       10.9889  100.0000    1.0000    0.0000    0.0000    2.7875    6.0000    0.0000
       -1.0000    0.0000   80.7000   34.9555    0.4988    0.0000    0.8563    0.0000
       -5.1872    3.1491    1.0000    4.0000    2.5791    0.0000    0.0000    0.0000
Cl      1.7140    1.0000   35.4500    1.9139    0.2000    0.3837   -1.0000    7.0000
       11.5345   10.1330    1.0000    0.0000    0.0000    9.9614    6.5316    0.0000
       -1.0000    3.5750  143.1770    6.2293    5.2294    0.1542    0.8563    0.0000
      -10.2080    2.9867    1.0338    6.2998    2.5791    0.0000    0.0000    0.0000
X      -0.0998    2.0000    1.0080    2.0000    0.0000    1.0000   -0.1000    6.0000
       10.0000    2.5000    4.0000    0.0000    0.0000    8.5000    1.5000    0.0000
       -0.1000    0.0000   -2.3700    8.7410   13.3640    0.6690    0.9745    0.0000
      -11.0000    2.7466    1.0338    4.0000    2.8793    0.0000    0.0000    0.0000
10        ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                              pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
 1   1 153.3934    0.0000    0.0000   -0.4600    0.0000    1.0000    6.0000    0.7300
           6.2500    1.0000    0.0000    1.0000   -0.0790    6.0552    0.0000    0.0000
 2   2 142.2858  145.0000   50.8293    0.2506   -0.1000    1.0000   29.7503    0.6051
           0.3451   -0.1055    9.0000    1.0000   -0.1225    5.5000    1.0000    0.0000
 1   2 160.0000    0.0000    0.0000   -0.5725    0.0000    1.0000    6.0000    0.5626
           1.1150    1.0000    0.0000    0.0000   -0.0920    4.2790    0.0000    0.0000
 1   3   0.0000    0.0000    0.0000    0.2000   -0.1418    1.0000   13.1260    0.5000
           0.5000   -0.2000   20.0000    1.0000   -0.1000    9.0000    0.0000    0.0000
 2   3  67.5157    0.0000    0.0000    0.6490   -0.3000    1.0000   36.0000    0.0625
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         0.4464   -0.2500   12.0000    1.0000   -0.0535    8.0407    0.0000    0.0000
 3   3  75.6595    0.0000    0.0000   -0.3638   -0.2000    0.0000   16.0000    0.2667
         0.6881   -0.2000   15.0000    1.0000   -0.1363    5.2877    0.0000    0.0000
 1   4 109.1686    0.0000    0.0000   -0.1657   -0.2000    0.0000   16.0000    1.2500
         2.8463   -0.2000   15.0000    1.0000   -0.1111    5.2687    0.0000    0.0000
 2   4   0.0000    0.0000    0.0000    0.5000   -0.2000    0.0000   16.0000    0.5000
         1.0001   -0.2000   15.0000    1.0000   -0.1000   10.0000    0.0000    0.0000
 3   4 118.3052    0.0000    0.0000   -0.1168   -0.2000    0.0000   16.0000    0.0697
         2.9176   -0.2000   15.0000    1.0000   -0.1316    5.3624    0.0000    0.0000
 4   4   0.2500    0.0000    0.0000    0.1803   -0.2000    0.0000   16.0000    0.3356
         0.9228   -0.2000   15.0000    1.0000   -0.1178    5.6715    0.0000    0.0000
 6      ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1   2   0.0283    1.2885   10.9190    0.9215   -1.0000   -1.0000
 1   3   0.0300    1.5200   12.5000    0.1000   -1.0000   -1.0000
 2   3   0.0277    1.6718   12.3537    1.7071   -1.0000   -1.0000
 1   4   0.0568    1.6740    9.6297    1.2200   -1.0000   -1.0000
 2   4   0.1927    2.2551   11.2308   -1.0000   -1.0000   -1.0000
 3   4   0.1402    2.1604   10.9786    1.7505   -1.0000   -1.0000
18      ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
 1   1   1    0.0000   27.9213    5.8635    0.0000    0.0000    0.0000    1.0400
 2   2   2   80.7324   30.4554    0.9953    0.0000    3.0000   50.0000    1.0783
 1   2   2   75.6935   50.0000    2.0000    0.0000    1.0000    0.0000    1.1680
 1   2   1   85.8000    9.8453    2.2720    0.0000    2.8635    0.0000    1.5800
 2   1   2    0.0000   15.0000    2.8900    0.0000    0.0000    0.0000    2.8774
 1   1   2    0.0000    8.5744    3.0000    0.0000    0.0000    0.0000    1.0421
 2   3   2 117.0684    0.0100   13.0091    0.0000    0.6109    0.0000    1.6252
 2   3   2   -7.1924    4.3581    3.5873    0.0000    0.8978    0.0000    1.5432
 3   2   3 114.2515    7.1068    6.8068    0.0000    0.1223    0.0000    2.6169
 1   2   3   55.0417    3.5032    3.9979    0.0000    1.5171    0.0000    1.0400
 2   2   3   76.3170   36.7758    2.7600    0.0000    1.2997    0.0000    1.1390
 2   3   3   56.7576   13.7652    0.8645    0.0000    1.3498    0.0000    1.2834
 2   3   4   96.6924    9.4823    5.7883    0.0000    0.2248    0.0000    2.2640
 2   3   4    0.0000    3.8549    3.7230    0.0000    0.1482    0.0000    1.0400
 3   4   3    0.0000   11.2336    6.8851    0.0000    1.0000    0.0000    1.0893
 3   3   4   90.0000    5.0811    5.2147    0.0000    1.0000    0.0000    1.8538
 4   3   4    0.0100   21.1482    0.3506    0.0000    1.0000    0.0000    1.4361
 2   1   4    0.0000    0.0100    0.5211    0.0000    0.0000    0.0000    1.3859
 7      ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1   2   2   2    0.8302   -4.0000   -0.7763   -2.5000   -1.0000    0.0000    0.0000
 2   2   2   2   -2.5000   -4.0000    1.0000   -2.5000   -1.0000    0.0000    0.0000
 0   1   1   0    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000
 0   1   2   0    0.0000    0.1000    0.0200   -2.5415    0.0000    0.0000    0.0000
 0   2   2   0    0.5511   25.4150    1.1330   -5.1903   -1.0000    0.0000    0.0000
 1   2   3   2   -1.5000    6.8333   -0.1978   -1.4683    0.0000    0.0000    0.0000
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1 2 3 4 0.1589 12.5000 0.4388 -1.5000 0.0000 0.0000 0.0000
1 ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
2 1 2 2.1200 -3.5800 1.4500 19.5000