Supplementary Information for "ReaxFF Reactive Force Field Modeling of the Triple-Phase Boundary in a Solid Oxide Fuel Cell"

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Reaction counts for selected reactions observed in 2 ns NVT simulation of butane decomposition and oxidation at YSZ/Ni interface at 2000 K.

Dehydration reactions

C_4H_x dehydration					Frequency
C_4H_{10}	→	C_4H_9	+	H	10
C_4H_9	→	C_4H_8	+	H	6
C_4H_8	→	C_4H_7	+	H	5
C_4H_7	→	C_4H_6	+	H	5
C_4H_6	→	C_4H_5	+	H	4
C_4H_5	→	C_4H_4	+	H	4
C_4H_4	→	C_4H_3	+	H	4
C_4H_3	→	C_4H_2	+	H	4
C_4H_2	→	C_4H	+	H	3
C_4H	→	C_4	+	H	2

C_3H_x dehydration					Frequency
C_3H_7	→	C_3H_6	+	H	1
C_3H_6	→	C_3H_5	+	H	2
C_3H_5	→	C_3H_4	+	H	3
C_3H_4	→	C_3H_3	+	H	3
C_3H_3	→	C_3H_2	+	H	4
C_3H_2	→	C_3H	+	H	3
C_3H	→	C_3	+	H	3

C_2H_x dehydration					Frequency
C_2H_6	→	C_2H_5	+	H	-1
C_2H_5	→	C_2H_4	+	H	2
C_2H_4	→	C_2H_3	+	H	5
C_2H_3	→	C_2H_2	+	H	5
C_2H_2	→	C_2H	+	H	5
C_2H	→	C_2	+	H	6

C-C bond cleavage reactions

C_4H_x C-C cleavage					Frequency
C_4H_{10}	→	C_3H_7	+	CH_3	2
C_4H_9	→	C_2H_5	+	C_2H_4	3
C_4H_9	→	C_3H_6	+	CH_3	1
C_4H_8	→	C_3H_5	+	CH_3	1
C_4H_6	→	C_3H_3	+	CH_3	1
C_4H_2	→	C_3	+	CH_2	1
C_4H	→	C_2H	+	C_2	1

C_3H_x C-C cleavage					Frequency
C_3H_7	→	C_2H_4	+	CH_3	1
C_3H_2	→	C_2	+	CH_2	1

C_2H_x C-C cleavage	Frequency
not observed	

Carbon-chain rearrangement reactions

C_x decomposition & addition							frequency
C_4			→	C_2	+	C_2	3
C_3	+	C_2	→	C_5			3
C_2	+	C	→	C_3			3
C_5	+	C_3	→	C_8			2
C_8			→	C_6	+	C_2	1
C_6			→	C_3	+	C_3	1
C_5	+	C	→	C_6			1
C_3	+	C	→	C_4			1
C_3	+	C	→	C_2	+	C_2	1
C_2			→	C	+	C	1

The Ni/YSZ ReaxFF developed by combining the YSZ and Ni/C/H descriptions and defining the missing angular terms from combination rules. Ni-Zr and Ni-Y bonded interactions were ignored; Ni/Y and Ni/Zr non-bonded parameters were obtained from combination rules.

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Reactive MD-force field; Cu, Ni, Co and all-carbon with Y/Zr/Ba
 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)
    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
 15    ! 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
 C    1.3817   4.0000  12.0000   1.8903   0.1838   0.9000   1.1341   4.0000
      9.7559   2.1346   4.0000  34.9350  79.5548   5.9666   7.0000   0.0000
      1.2114   0.0000 202.6057   8.9539  34.9289  13.5366   0.8563   0.0000
     -2.8983   2.5000   1.0564   4.0000   2.9663   0.0000   0.0000   0.0000
 H    0.7842   1.0000   1.0080   1.4029   0.0420   0.9177  -0.1000   1.0000
      9.2018   5.0518   1.0000   0.0000 121.1250   5.2155   8.9069   1.0000
     -0.1000   0.0000  61.6232   2.0650   2.9910   0.6549   1.0698   0.0000
    -15.7683   2.1488   1.0338   1.0000   2.8793   0.0000   0.0000   0.0000
 O    1.2477   2.0000  15.9990   1.9236   0.0904   1.0503   1.0863   6.0000
     10.2127   7.7719   4.0000  36.9573 116.0768   8.5000   8.9989   2.0000
      0.9088   1.0003  60.8726  20.4140   3.3754   0.2702   0.9745   0.0000
     -3.6141   2.7025   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
 N    1.2333   3.0000  14.0000   1.9324   0.1376   0.8596   1.1748   5.0000
     10.0667   7.8431   4.0000  32.2482 100.0000   6.8418   6.3404   2.0000
      1.0433  13.7673 119.9837   2.1961   3.0696   2.7683   0.9745   0.0000
     -4.3875   2.6192   1.0183   4.0000   2.8793   0.0000   0.0000   0.0000
 S    1.9405   2.0000  32.0600   2.0677   0.2099   1.0336   1.5479   6.0000
      9.9575   4.9055   4.0000  52.9998 112.1416   6.5000   8.2545   2.0000
      1.4601   9.7177  71.1843   5.7487  23.2859  12.7147   0.9745   0.0000
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   -11.0000   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
Si   2.0132   4.0000  28.0600   2.2203   0.1306   0.8218   1.5629   4.0000
    12.1305   1.8838   4.0000  11.4056 139.9309   1.8038   7.3852   0.0000
    -1.0000   0.0000 128.2031   6.2293   5.2294   0.1542   0.8563   0.0000
    -3.6886   2.9867   1.0338   4.0000   2.5791   0.0000   0.0000   0.0000
Pt   1.9907   3.0000 195.0800   1.9980   0.2452   0.8218  -1.0000   3.0000
    12.8669   3.2118   3.0000   0.0000   0.0000   1.8038   7.3852   0.0000
    -1.0000   0.0000 143.1770   6.2293   5.2294   0.1542   0.8563   0.0000
    -6.7740   2.9867   1.0338   3.0000   2.5791   0.0000   0.0000   0.0000
Zr   2.1000   4.0000  91.2240   2.1970   0.2542   0.8218  -1.0000   4.0000
    12.8545   3.5938   4.0000   0.0000   0.0000   1.8038   7.3852   0.0000
    -1.0000   0.0000 143.1770   6.2293   5.2294   0.1542   0.8563   0.0000
    -3.2224   2.9867   1.0338   4.0000   2.5791   0.0000   0.0000   0.0000
Ni   1.9384   2.0000  58.6900   1.9565   0.1590   0.8218   0.1000   2.0000
    12.1088   3.8387   2.0000   0.0000   0.0000   4.8038   7.3852   0.0000
    -1.0000   0.0000 102.0350  16.0205   4.1150   0.1116   0.8563   0.0000
    -3.7733   4.8815   1.0338   8.0000   2.5791   0.0000   0.0000   0.0000
Cu   1.9178   1.0000  63.5460   1.9554   0.1621   0.8218   0.1000   1.0000
    12.2407   4.2220   1.0000   0.0000   0.0000   4.8038   7.3852   0.0000
    -1.0000   0.0000  92.5070   6.2293   5.2294   0.1542   0.8563   0.0000
    -3.2224   2.9867   1.0338   1.0000   2.5791   0.0000   0.0000   0.0000
Co   2.0075   3.0000  58.9332   1.8480   0.2056   0.8218   0.1000   3.0000
    12.3582   3.4682   3.0000   0.0000   0.0000   4.8038   7.3852   0.0000
    -1.0000   0.0000  92.5070   6.2293   5.2294   0.1542   0.8563   0.0000
    -3.3353   2.9867   1.0338   3.0000   2.5791   0.0000   0.0000   0.0000
Zr   2.6606   4.0000  91.2240   2.2821   0.2556   0.7127  -1.0000   4.0000
    11.5975  48.3221   4.0000  -5.0000   0.0000  -2.7483   6.0000   0.0000
    -1.0000   0.0000 144.6080  48.1308   0.0807   0.0000   0.8563   0.0000
    -7.4872   3.3675   1.0338   8.0000   2.2632   0.0000   0.0000   0.0000
Y    2.7444   3.0000  88.9052   2.4847   0.3051   0.3696  -1.0000   3.0000
    11.7782  49.8808   3.0000  -5.0000   0.0000  -4.5000   6.0000   0.0000
    -1.0000   0.0000 100.3750  59.9971  74.9975   0.0000   0.8563   0.0000
    -2.6125   2.9867   1.0338   3.0000   2.5791   0.0000   0.0000   0.0000
Ba   2.5719   2.0000 137.3270   2.6981   0.2997   0.4585  -1.0000   2.0000
    10.3886  47.5071   2.0000  -5.0000   0.0000  -5.6022   5.5467   0.0000
    -1.0000   0.0000 143.1770 109.4891   9.4011   0.0147   0.8563   0.0000
    -7.4827   2.9867   1.0338   2.0000   2.5791   0.0000   0.0000   0.0000
X   -0.1000   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   6.2998   2.8793   0.0000   0.0000   0.0000
47      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                       pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
 1  1 158.2004  99.1897  78.0000  -0.7738  -0.4550   1.0000  37.6117   0.4147
       0.4590  -0.1000   9.1628   1.0000  -0.0777   6.7268   1.0000   0.0000
 1  2 169.4760   0.0000   0.0000  -0.6083   0.0000   1.0000   6.0000   0.7652
       5.2290   1.0000   0.0000   1.0000  -0.0500   6.9136   0.0000   0.0000
 2  2 145.0803   0.0000   0.0000  -0.4173   0.0000   1.0000   6.0000   1.0000
       5.2125   1.0000   0.0000   1.0000  -0.0472   4.0758   0.0000   0.0000
 1  3 160.4802 105.1693  23.3059  -0.3873  -0.1613   1.0000  10.8851   1.0000
       0.5341  -0.3174   7.0303   1.0000  -0.1463   5.2913   0.0000   0.0000
 3  3  60.1463 176.6202  51.1430  -0.2802  -0.1244   1.0000  29.6439   0.9114
       0.2441  -0.1239   7.6487   1.0000  -0.1302   6.2919   1.0000   0.0000
 1  4 134.1215 140.2179  79.9745   0.0163  -0.1428   1.0000  27.0617   0.2000
       0.1387  -0.3681   7.1611   1.0000  -0.1000   5.0825   1.0000   0.0000
 3  4 130.8596 169.4551  40.0000   0.3837  -0.1639   1.0000  35.0000   0.2000
       1.0000  -0.3579   7.0004   1.0000  -0.1193   6.8773   1.0000   0.0000
 4  4 157.9384  82.5526 152.5336   0.4010  -0.1034   1.0000  12.4261   0.5828
       0.1578  -0.1509  11.9186   1.0000  -0.0861   5.4271   1.0000   0.0000
 2  3 180.4373   0.0000   0.0000  -0.8074   0.0000   1.0000   6.0000   0.5514
       1.2490   1.0000   0.0000   1.0000  -0.0657   5.0451   0.0000   0.0000
 2  4 231.8173   0.0000   0.0000  -0.3364   0.0000   1.0000   6.0000   0.4402
       8.8910   1.0000   0.0000   1.0000  -0.0327   6.5754   0.0000   0.0000
 1  5 128.9942  74.5848  55.2528   0.1035  -0.5211   1.0000  18.9617   0.6000
       0.2949  -0.2398   8.1175   1.0000  -0.1029   5.6731   1.0000   0.0000
 2  5 151.5159   0.0000   0.0000  -0.4721   0.0000   1.0000   6.0000   0.6000
       9.4366   1.0000   0.0000   1.0000  -0.0290   7.0050   1.0000   0.0000
 3  5   0.0000   0.0000   0.0000   0.5563  -0.4038   1.0000  49.5611   0.6000
       0.4259  -0.4577  12.7569   1.0000  -0.1100   7.1145   1.0000   0.0000
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 4  5   0.0000   0.0000   0.0000   0.4438  -0.2034   1.0000  40.3399   0.6000
         0.3296  -0.3153   9.1227   1.0000  -0.1805   5.6864   1.0000   0.0000
 5  5  96.1871  93.7006  68.6860   0.0955  -0.4781   1.0000  17.8574   0.6000
         0.2723  -0.2373   9.7875   1.0000  -0.0950   6.4757   1.0000   0.0000
 6  6 113.7903  53.9894  30.0000   0.2535  -0.3000   1.0000  16.0000   0.0742
         0.2586  -0.1963   7.5407   1.0000  -0.0693   7.9365   0.0000   0.0000
 2  6 138.8626   0.0000   0.0000  -0.1577   0.0000   1.0000   6.0000   0.2901
        17.8821   1.0000   0.0000   1.0000  -0.0395   6.3931   0.0000   0.0000
 3  6 193.1177  41.1424  43.3991  -0.2085  -0.3000   1.0000  36.0000   0.7695
         0.9220  -0.3683   4.2644   1.0000  -0.5191   4.4529   1.0000   0.0000
 4  6 185.4488  39.2832  43.3991  -0.1922  -0.3000   1.0000  36.0000   0.8217
         0.8538  -0.3887   4.4334   1.0000  -0.5241   4.4529   1.0000   0.0000
 7  7  90.1462   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.3484
         1.0000  -0.2000  15.0000   1.0000  -0.1014   5.7631   0.0000   0.0000
 8  8  85.2900   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.5438
         1.0000  -0.2000  15.0000   1.0000  -0.1001   5.5699   0.0000   0.0000
 1  9  75.3001  14.9046   0.0000   0.5121  -0.2000   1.0000  16.0000   0.1231
         0.5004  -0.1126  12.4658   1.0000  -0.1123   5.2695   1.0000   0.0000
 2  9 115.3598   0.0000   0.0000   0.7039   0.0000   1.0000   6.0000   0.1029
         0.0928   1.0000   0.0000   1.0000  -0.1505   4.9690   0.0000   0.0000
 3  9 130.2089   0.0000   0.0000  -0.0843  -0.2000   1.0000  16.0000   0.1845
         0.8022  -0.2500  15.0000   1.0000  -0.1189   5.8835   1.0000   0.0000
 9  9  87.8565   0.0000   0.0000  -0.2420  -0.2000   0.0000  16.0000   0.3215
         1.2270  -0.2000  15.0000   1.0000  -0.1242   5.0785   0.0000   0.0000
 1 10  89.6936   5.9366   0.0000   0.1026  -0.2000   1.0000  16.0000   0.4912
         0.7370  -0.2309   9.2387   1.0000  -0.1086   6.1689   1.0000   0.0000
 2 10  73.6182   0.0000   0.0000  -0.5004  -0.2000   0.0000  16.0000   0.3418
         9.0000  -0.2000  15.0000   1.0000  -0.1015   5.7850   0.0000   0.0000
10 10  70.2770   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.3424
         1.0000  -0.2000  15.0000   1.0000  -0.1098   6.1263   0.0000   0.0000
 1 11  83.8766   7.6132   0.0000   0.1332  -0.2000   1.0000  16.0000   0.2308
         0.7624  -0.2167   7.4106   1.0000  -0.1291   5.2562   1.0000   0.0000
 2 11  73.6182   0.0000   0.0000  -0.5004  -0.2000   0.0000  16.0000   0.3418
         9.0000  -0.2000  15.0000   1.0000  -0.1015   5.7850   0.0000   0.0000
11 11  68.1504   0.0000   0.0000  -0.4743  -0.2000   0.0000  16.0000   0.2865
         1.3468  -0.2000  15.0000   1.0000  -0.0596   8.1864   0.0000   0.0000
12 12  76.6674   0.0000   0.0000  -0.1508  -0.2000   0.0000  16.0000   0.3630
         0.8019  -0.2000  15.0000   1.0000  -0.1682   6.4675   0.0000   0.0000
 3 12 112.7221   0.0000   0.0000   0.4102  -0.3000   1.0000  36.0000   0.3592
         0.1355  -0.2000  15.0000   1.0000  -0.1016  10.6210   1.0000   0.0000
 2 12  38.8626   0.0000   0.0000  -0.1577   0.0000   1.0000   6.0000   0.5000
        17.8821   1.0000   0.0000   1.0000  -0.2095   6.3931   0.0000   0.0000
13 13  67.0143   0.0000   0.0000  -0.2340  -0.2000   0.0000  16.0000   0.3587
         1.3169  -0.2000  15.0000   1.0000  -0.0617   7.1124   0.0000   0.0000
 3 13 135.5054   0.0000   0.0000   0.1864  -0.3000   1.0000  36.0000   0.7491
         0.3112  -0.2000  15.0000   1.0000  -0.1194   7.4818   1.0000   0.0000
 2 13  38.8626   0.0000   0.0000  -0.1577   0.0000   1.0000   6.0000   0.2901
        17.8821   1.0000   0.0000   1.0000  -0.2095   6.3931   0.0000   0.0000
12 13  68.4867   0.0000   0.0000  -0.1337  -0.2000   0.0000  16.0000   0.4185
         0.3865  -0.2000  15.0000   1.0000  -0.0949   7.2021   0.0000   0.0000
 3 14  27.7578   0.0000   0.0000  -0.6396  -0.3000   1.0000  36.0000   0.1964
         0.5934  -0.2000  15.0000   1.0000  -0.0500   6.9774   1.0000   0.0000
 2 14  38.8626   0.0000   0.0000  -0.1577   0.0000   1.0000   6.0000   0.2901
        17.8821   1.0000   0.0000   1.0000  -0.2095   6.3931   0.0000   0.0000
12 14  86.8034   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.2619
         1.0000  -0.2000  15.0000   1.0000  -0.0650   5.4900   0.0000   0.0000
13 14  21.4666   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.6381
         1.0000  -0.2000  15.0000   1.0000  -0.1464   9.2410   0.0000   0.0000
14 14  29.0409   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.4045
         1.0000  -0.2000  15.0000   1.0000  -0.0455   5.2968   0.0000   0.0000
 9 12  66.5036   0.0000   0.0000  -0.1234  -0.2000   0.0000  16.0000   0.2118
         0.8409  -0.2000  15.0000   1.0000  -0.1862   6.3438   0.0000   0.0000
 9 13  54.8641   0.0000   0.0000  -0.0373  -0.2000   0.0000  16.0000   0.2562
         0.6361  -0.2000  15.0000   1.0000  -0.1974   6.5566   0.0000   0.0000
 1 12   0.0000   0.0000   0.0000  -0.2500   0.0000   1.0000   6.0000   0.5000
         1.0000   1.0000   0.0000   1.0000  -0.2000  10.0000   0.0000   0.0000
 1 13   0.0000   0.0000   0.0000  -0.2500   0.0000   1.0000   6.0000   0.5000
         1.0000   1.0000   0.0000   1.0000  -0.2000  10.0000   0.0000   0.0000
25    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
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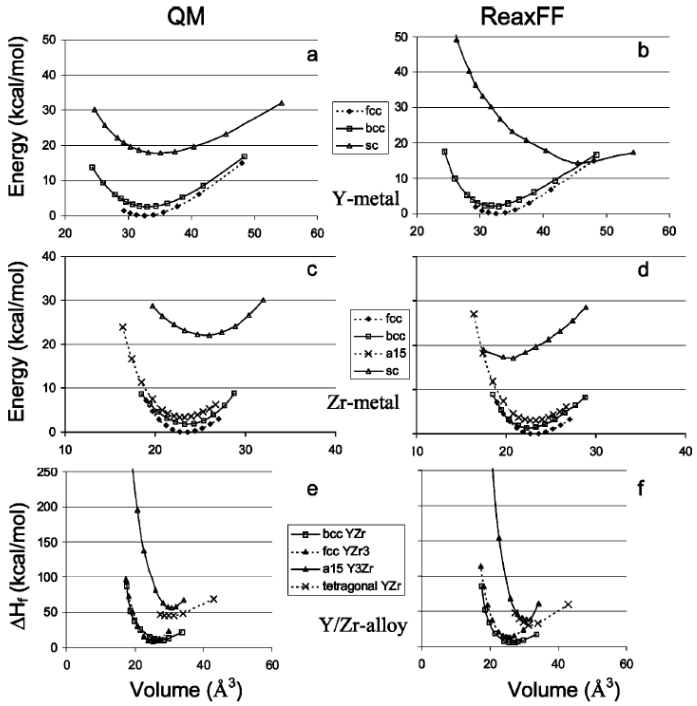
  1  2   0.1239   1.4004   9.8467   1.1210  -1.0000  -1.0000
  2  3   0.0344   1.6800  10.3247   0.9013  -1.0000  -1.0000
  2  4   0.1059   1.8290   9.7818   0.9598  -1.0000  -1.0000
  1  3   0.1131   1.8523   9.8442   1.2775   1.1342   1.0621
  1  4   0.1447   1.8766   9.7990   1.3436   1.1885   1.1363
  3  4   0.1048   2.0003  10.1220   1.3173   1.1096   1.0206
  2  6   0.0456   1.6477  12.2823   1.1654  -1.0000  -1.0000
  3  6   0.1233   1.7552  10.6931   1.6096   1.2935  -1.0000
  4  6   0.1316   1.9463  11.1198   1.7196   1.4858  -1.0000
  1  9   0.1836   1.6009  10.0711   1.6605   1.3974  -1.0000
  2  9   0.0446   1.6704  11.8699   1.2420  -1.0000  -1.0000
  3  9   0.0677   1.8010  11.7855   1.4585  -1.0000  -1.0000
  1 10   0.0813   1.7091  11.9584   1.5703   1.3629  -1.0000
  1 11   0.0879   1.7302  11.8588   1.4583   1.4235  -1.0000
  3 12   0.1570   1.7138  12.0409   1.9449  -1.0000  -1.0000
  3 13   0.2151   1.7134  13.0000   1.8219  -1.0000  -1.0000
  2 12   0.1000   1.7610  10.4809   0.1000  -1.0000  -1.0000
  2 13   0.1000   1.7610  10.4809   0.1000  -1.0000  -1.0000
 12 13   0.2975   2.2017  12.2223   2.5808  -1.0000  -1.0000
  2 14   0.1000   1.7610  10.4809   0.1000  -1.0000  -1.0000
  3 14   0.2983   1.7480  12.9975   2.1772  -1.0000  -1.0000
 12 14   0.2979   2.5544  13.0000   2.4544  -1.0000  -1.0000
 13 14   0.2279   2.1441  11.3571   2.5038  -1.0000  -1.0000
  9 12   0.2330   2.2569  11.1199   2.3048  -1.0000  -1.0000
  9 13   0.2539   2.2551  11.1902   2.2979  -1.0000  -1.0000
113    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2;val(bo)
  1  1  1  59.0573  30.7029   0.7606   0.0000   0.7180   6.2933   1.1244
  1  1  2  65.7758  14.5234   6.2481   0.0000   0.5665   0.0000   1.6255
  2  1  2  70.2607  25.2202   3.7312   0.0000   0.0050   0.0000   2.7500
  1  2  2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000   1.0400
  1  2  1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000   1.0400
  2  2  2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000   1.0400
  1  1  3  49.5561   7.3771   4.9568   0.0000   0.7533  15.9906   1.0010
  3  1  3  77.1171  39.8746   2.5403 -24.3902   1.7740 -42.9758   2.1240
  1  1  4  66.1305  12.4661   7.0000   0.0000   3.0000  50.0000   1.1880
  3  1  4  73.9544  12.4661   7.0000   0.0000   3.0000   0.0000   1.1880
  4  1  4  64.1581  12.4661   7.0000   0.0000   3.0000   0.0000   1.1880
  2  1  3  65.0000  14.2057   4.8649   0.0000   0.3504   0.0000   1.7185
  2  1  4  74.2929  31.0883   2.6184   0.0000   0.0755   0.0000   1.0500
  1  2  4   0.0000   0.0019   6.3000   0.0000   0.0000   0.0000   1.0400
  1  3  1  74.3994  44.7500   0.7982   0.0000   3.0000   0.0000   1.0528
  1  3  3  77.9854  36.6201   2.0201   0.0000   0.7434  67.0264   3.0000
  1  3  4  82.4890  31.4554   0.9953   0.0000   1.6310   0.0000   1.0783
  3  3  3  80.7324  30.4554   0.9953   0.0000   1.6310  50.0000   1.0783
  3  3  4  84.3637  31.4554   0.9953   0.0000   1.6310   0.0000   1.0783
  4  3  4  89.7071  31.4554   0.9953   0.0000   1.6310   0.0000   1.1519
  1  3  2  71.5018  21.7062   0.4735   0.0000   0.5186   0.0000   1.1793
  2  3  3  84.9468  23.3540   1.5057   0.0000   2.6374   0.0000   1.3023
  2  3  4  75.6201  18.7919   0.9833   0.0000   0.1218   0.0000   1.0500
  2  3  2  77.0645  10.4737   1.2895   0.0000   0.9924   0.0000   1.1043
  1  4  1  66.0330  22.0295   1.4442   0.0000   1.6777   0.0000   1.0500
  1  4  3 103.3204  33.0381   0.5787   0.0000   1.6777   0.0000   1.0500
  1  4  4 104.1335   8.6043   1.6495   0.0000   1.6777   0.0000   1.0500
  3  4  3  74.1978  42.1786   1.7845 -18.0069   1.6777   0.0000   1.0500
  3  4  4  74.8600  43.7354   1.1572  -0.9193   1.6777   0.0000   1.0500
  4  4  4  75.0538  14.8267   5.2794   0.0000   1.6777   0.0000   1.0500
  1  4  2  69.1106  25.5067   1.1003   0.0000   0.0222   0.0000   1.0369
  2  4  3  81.3686  40.0712   2.2396   0.0000   0.0222   0.0000   1.0369
  2  4  4  83.0104  43.4766   1.5328   0.0000   0.0222   0.0000   1.0500
  2  4  2  70.8687  12.0168   5.0132   0.0000   0.0222   0.0000   1.1243
  1  2  3   0.0000  25.0000   3.0000   0.0000   1.0000   0.0000   1.0400
  1  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
  1  2  5   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
  3  2  3   0.0000   0.0148   6.0000   0.0000   0.0000   0.0000   1.0400
  3  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
  4  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
  2  2  3   0.0000   9.7025   6.0000   0.0000   0.0000   0.0000   1.0400
  2  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
  1  1  5  74.9397  25.0560   1.8787   0.1463   0.0559   0.0000   1.0400
```

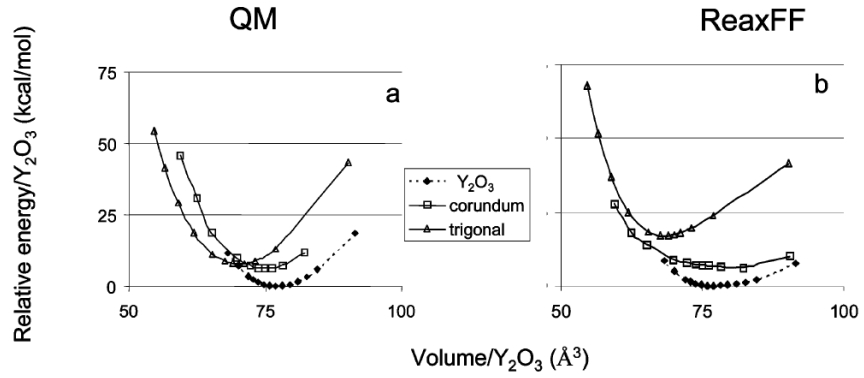
1	5	1	86.9521	36.9951	2.0903	0.1463	0.0559	0.0000	1.0400
2	1	5	74.9397	25.0560	1.8787	0.0000	0.0000	0.0000	1.0400
1	5	2	86.1791	36.9951	2.0903	0.0000	0.0000	0.0000	1.0400
1	5	5	85.3644	36.9951	2.0903	0.1463	0.0559	0.0000	1.0400
2	5	2	93.1959	36.9951	2.0903	0.0000	0.0000	0.0000	1.0400
2	5	5	84.3331	36.9951	2.0903	0.0000	0.0000	0.0000	1.0400
6	6	6	69.3456	21.7361	1.4283	0.0000	-0.2101	0.0000	1.3241
2	6	6	75.6168	21.5317	1.0435	0.0000	2.5179	0.0000	1.0400
2	6	2	78.3939	20.9772	0.8630	0.0000	2.8421	0.0000	1.0400
3	6	6	70.3016	15.4081	1.3267	0.0000	2.1459	0.0000	1.0400
2	6	3	73.8232	16.6592	3.7425	0.0000	0.8613	0.0000	1.0400
3	6	3	90.0344	7.7656	1.7264	0.0000	0.7689	0.0000	1.0400
6	3	6	22.1715	3.6615	0.3160	0.0000	4.1125	0.0000	1.0400
2	3	6	83.7634	5.6693	2.7780	0.0000	1.6982	0.0000	1.0400
3	3	6	73.4663	25.0761	0.9143	0.0000	2.2466	0.0000	1.0400
2	2	6	0.0000	47.1300	6.0000	0.0000	1.6371	0.0000	1.0400
6	2	6	0.0000	31.5209	6.0000	0.0000	1.6371	0.0000	1.0400
3	2	6	0.0000	31.0427	4.5625	0.0000	1.6371	0.0000	1.0400
4	6	6	64.4297	13.1239	1.1830	0.0000	2.1459	0.0000	1.0400
4	6	4	78.4992	7.8594	2.3011	0.0000	0.7689	0.0000	1.0400
3	6	4	77.4641	4.5724	1.0849	0.0000	0.7689	0.0000	1.0400
6	4	6	25.5269	3.0725	0.2486	0.0000	4.1125	0.0000	1.0400
2	6	4	77.4079	16.0992	2.2665	0.0000	0.8613	0.0000	1.0400
2	4	6	74.6462	4.7671	1.6524	0.0000	1.6982	0.0000	1.0400
4	4	6	76.8202	12.7851	0.6196	0.0000	2.2466	0.0000	1.0400
3	4	6	69.8728	32.7155	1.5875	0.0000	2.2466	0.0000	1.0400
4	3	6	69.8728	27.1273	1.5875	0.0000	2.2466	0.0000	1.0400
4	2	6	0.0000	31.0427	4.5625	0.0000	1.6371	0.0000	1.0400
1	10	1	78.3532	39.1762	2.5455	0.0000	0.8059	0.0000	0.9983
1	1	10	45.4463	15.9209	1.6664	0.0000	0.0217	0.0000	1.0282
1	11	1	84.6882	18.1124	1.0794	0.0000	1.7791	0.0000	1.8728
1	1	11	36.1871	8.8505	5.3270	0.0000	1.7712	0.0000	1.7983
1	9	1	70.5162	40.5170	0.6074	0.0000	1.5553	0.0000	1.9312
1	1	9	89.8137	28.5641	0.2698	0.0000	0.0100	0.0000	1.0400
9	1	9	88.0856	19.2144	7.0000	0.0000	0.0100	0.0000	2.0481
1	9	9	44.3880	1.9725	0.1392	0.0000	0.0877	0.0000	2.5527
3	9	3	60.0013	22.1615	1.9291	0.0000	0.0578	0.0000	1.2775
3	3	9	90.0000	31.1442	5.0000	0.0000	0.5686	0.0000	2.0931
9	3	9	37.1692	2.8761	1.2192	0.0000	1.3131	0.0000	1.1000
3	9	9	75.5003	2.8573	2.4899	0.0000	0.7658	0.0000	2.6141
2	9	2	105.7916	13.3105	2.8991	0.0000	1.3744	0.0000	1.5788
2	2	9	0.0000	34.4450	5.0000	0.0000	2.0000	0.0000	1.8492
9	2	9	0.0000	59.5562	4.9736	0.0000	2.0000	0.0000	1.5094
2	9	9	47.7079	4.1085	1.3292	0.0000	0.3651	0.0000	4.0000
2	9	9	180.0000	-34.4237	16.4333	0.0000	0.8112	0.0000	1.5285
1	9	2	74.4441	0.1000	2.0522	0.5000	1.2749	0.0000	2.8183
1	2	9	0.0000	0.1000	1.4854	0.0000	1.1641	0.0000	2.3023
2	1	9	39.0776	16.2074	2.1899	0.5000	0.0649	0.0000	1.0405
2	3	9	60.5811	18.7714	2.1925	0.5000	0.0500	0.0000	1.1000
1	9	3	70.0000	25.0000	1.0000	0.0000	1.0000	0.0000	1.2500
1	3	9	70.0000	25.0000	1.0000	0.0000	1.0000	0.0000	1.2500
3	1	9	70.0000	25.0000	1.0000	0.0000	1.0000	0.0000	1.2500
3	2	9	0.0000	7.1233	1.9895	0.5000	0.3233	0.0000	1.1000
2	3	12	42.5058	10.0776	5.0000	0.0000	0.9289	0.0000	1.1912
2	3	13	50.0000	4.9111	1.0014	0.0000	1.0000	0.0000	1.1000
2	3	14	90.0000	4.4647	1.6312	0.0000	1.0000	0.0000	1.1000
3	12	3	52.5575	19.0581	0.4111	0.0000	0.1000	0.0000	1.4556
3	13	3	54.7233	20.0000	3.9000	0.0000	2.9687	0.0000	2.2203
3	14	3	96.7972	3.1674	4.0000	0.0000	0.2351	0.0000	1.1538
12	3	12	8.3158	7.8049	0.2315	0.0000	2.2934	0.0000	3.0000
12	3	13	6.8406	0.1375	0.2897	0.0000	0.2695	0.0000	2.8046
13	3	13	1.3950	3.4274	7.5393	0.0000	2.2693	0.0000	1.1000
12	3	14	64.7868	4.2318	2.8328	0.0000	1.6405	0.0000	1.3967
13	3	14	82.6362	1.8110	1.9414	0.0000	1.3074	0.0000	2.3916
14	3	14	59.1887	3.0968	2.3507	0.0000	1.8482	0.0000	1.3745
3	3	12	80.0000	10.0000	1.2500	0.0000	0.5554	0.0000	1.2000
3	3	13	80.0000	25.0000	1.2500	0.0000	0.5554	0.0000	1.2000
3	3	14	80.0000	15.0000	1.2500	0.0000	0.5554	0.0000	1.2000
9	3	12	21.3736	2.6570	0.8220	0.0000	2.0000	0.0000	1.2756

```
 9  3 13  18.7146  10.3571   3.4779   0.0000   1.9121   0.0000   1.1848
51    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1  1  1  1  -0.2500  34.7453   0.0288  -6.3507  -1.6000   0.0000   0.0000
 1  1  1  2  -0.2500  29.2131   0.2945  -4.9581  -2.1802   0.0000   0.0000
 2  1  1  2  -0.2500  31.2081   0.4539  -4.8923  -2.2677   0.0000   0.0000
 1  1  1  3  -0.7098  22.2951   0.0060  -2.5000  -2.1688   0.0000   0.0000
 2  1  1  3  -0.3568  22.6472   0.6045  -4.0088  -1.0000   0.0000   0.0000
 3  1  1  3  -0.0528   6.8150   0.7498  -5.0913  -1.0000   0.0000   0.0000
 1  1  3  1   2.0007  25.5641  -0.0608  -2.6456  -1.1766   0.0000   0.0000
 1  1  3  2  -1.1953  42.1545  -1.0000  -8.0821  -1.0000   0.0000   0.0000
 2  1  3  1  -0.9284  34.3952   0.7285  -2.5440  -2.4641   0.0000   0.0000
 2  1  3  2  -2.5000  79.6980   1.0000  -3.5697  -2.7501   0.0000   0.0000
 1  1  3  3  -0.0179   5.0603  -0.1894  -2.5000  -2.0399   0.0000   0.0000
 2  1  3  3  -0.5583  80.0000   1.0000  -4.4000  -3.0000   0.0000   0.0000
 3  1  3  1  -2.5000  76.0427  -0.0141  -3.7586  -2.9000   0.0000   0.0000
 3  1  3  2   0.0345  78.9586  -0.6810  -4.1777  -3.0000   0.0000   0.0000
 3  1  3  3  -2.5000  66.3525   0.3986  -3.0293  -3.0000   0.0000   0.0000
 1  3  3  1   2.5000  -0.5332   1.0000  -3.5096  -2.9000   0.0000   0.0000
 1  3  3  2  -2.5000   3.3219   0.7180  -5.2021  -2.9330   0.0000   0.0000
 2  3  3  2   2.2500  -6.2288   1.0000  -2.6189  -1.0000   0.0000   0.0000
 1  3  3  3   0.0531 -17.3983   1.0000  -2.5000  -2.1584   0.0000   0.0000
 2  3  3  3   0.4723 -12.4144  -1.0000  -2.5000  -1.0000   0.0000   0.0000
 3  3  3  3  -2.5000 -25.0000   1.0000  -2.5000  -1.0000   0.0000   0.0000
 0  1  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  2  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  1  1  0   0.0000  50.0000   0.3000  -4.0000  -2.0000   0.0000   0.0000
 0  3  3  0   0.5511  25.4150   1.1330  -5.1903  -1.0000   0.0000   0.0000
 0  1  4  0  -2.4242 128.1636   0.3739  -6.6098  -2.0000   0.0000   0.0000
 0  2  4  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  3  4  0   1.4816  55.6641   0.0004  -7.0465  -2.7831   0.0000   0.0000
 0  4  4  0  -0.3244  27.7086   0.0039  -2.8272  -2.0000   0.0000   0.0000
 4  1  4  4  -5.5181   8.9706   0.0004  -6.1782  -2.0000   0.0000   0.0000
 0  1  5  0   3.3423  30.3435   0.0365  -2.7171   0.0000   0.0000   0.0000
 0  5  5  0  -0.0555 -42.7738   0.1515  -2.2056   0.0000   0.0000   0.0000
 0  2  5  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  6  6  0   0.0000   0.0000   0.1200  -2.4426   0.0000   0.0000   0.0000
 0  2  6  0   0.0000   0.0000   0.1200  -2.4847   0.0000   0.0000   0.0000
 0  3  6  0   0.0000   0.0000   0.1200  -2.4703   0.0000   0.0000   0.0000
 2  1  3 14   1.6297  56.8132   0.3398  -2.6912  -2.1000   0.0000   0.0000
 1  1  3 14  -0.0427  13.4096   0.9351  -6.5245  -2.1000   0.0000   0.0000
 2  3 14  3   2.5000  11.6208   1.0000  -9.0000  -1.0000   0.0000   0.0000
 2  1  3 12  -0.2500  45.7639   0.3000  -3.5745  -2.1565   0.0000   0.0000
 1  1  3 12  -0.2500  69.1094   0.3000  -3.0983  -2.1565   0.0000   0.0000
 2  3 12  3  -0.4306   7.5000  -0.5000  -6.9948  -1.0000   0.0000   0.0000
 2  3 11  3   1.8627   9.7180  -1.0000  -7.2224  -1.0000   0.0000   0.0000
 1  3 11  3   2.5000  23.9443   1.0000  -3.2267  -1.0000   0.0000   0.0000
 1  1  3 11   0.9114  62.5039  -0.2389  -3.2976  -1.0000   0.0000   0.0000
 2  1  3 11   0.5000  35.0000   0.5000  -4.0000  -1.0000   0.0000   0.0000
 1  1  1  9   0.1109  33.5901  -0.7768  -4.2047   0.0000   0.0000   0.0000
 9  1  1  9   0.0509  16.5248  -1.9621  -3.0000   0.0000   0.0000   0.0000
 2  1  1  9   1.2085  -2.0000   1.3837  -4.0804   0.0000   0.0000   0.0000
 9  3  3  9   0.0509  30.0000   0.5000  -4.0000   0.0000   0.0000   0.0000
 9    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
 3  2  3   1.9682  -4.4628   1.7976   3.0000
 3  2  4   2.0000  -6.0000   1.7976   3.0000
 4  2  3   1.2000  -2.0000   1.7976   3.0000
 4  2  4   1.2979  -6.0000   1.7976   3.0000
 3  2  5   1.5000  -2.0000   1.7976   3.0000
 4  2  5   1.5000  -2.0000   1.7976   3.0000
 5  2  3   1.5000  -2.0000   1.7976   3.0000
 5  2  4   1.5000  -2.0000   1.7976   3.0000
 5  2  5   1.5000  -2.0000   1.7976   3.0000
```

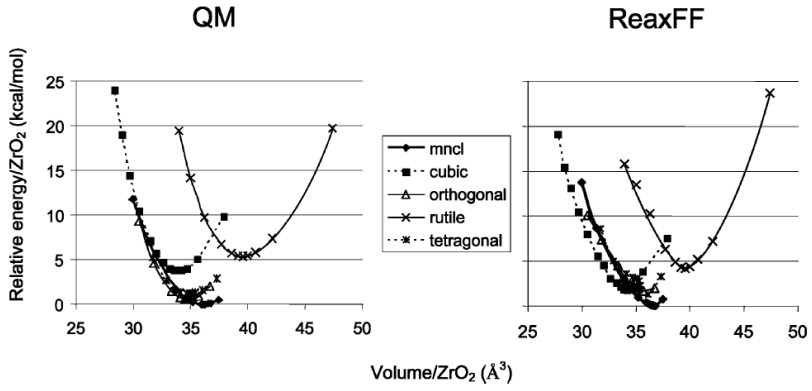
Examples of ReaxFF *vs.* QM energetics



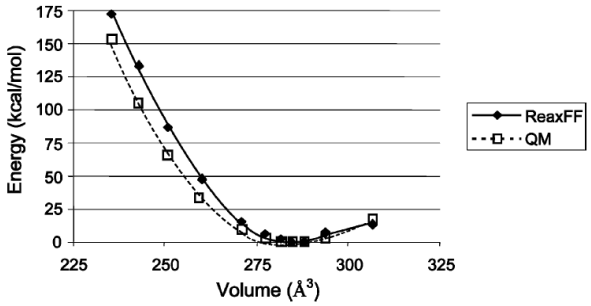
QM- and ReaxFF equations of state for various polymorphs of the Y metal (a,b), Zr metal (c, d) and Y/Zr alloys (e, f).[5]



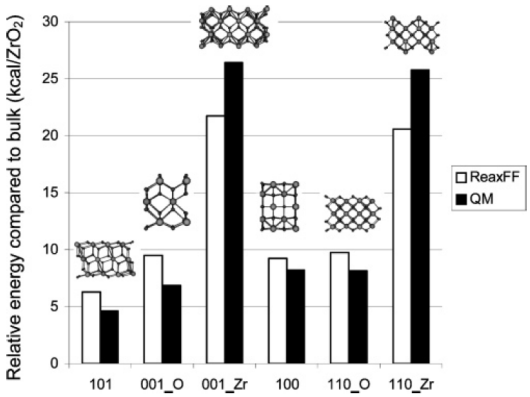
QM- and ReaxFF equations of state for various polymorphs of Y_2O_3.[5]



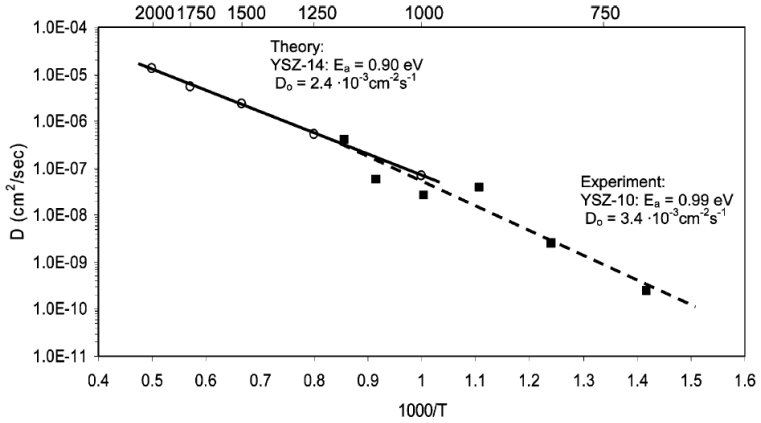
QM- and ReaxFF equations of state for polymorphs of ZrO_2.[5]



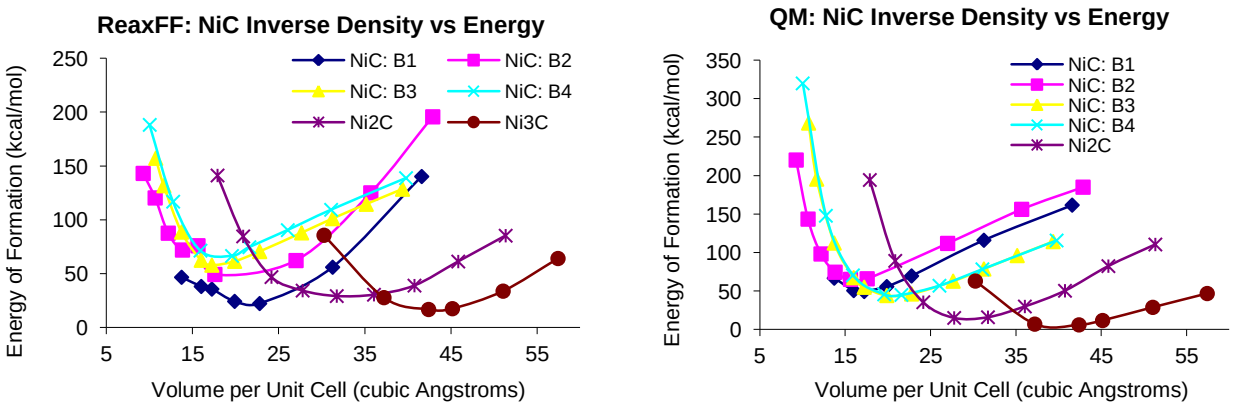
QM- and ReaxFF equations of state for a YSZ-14 phase $[(Y_2O_3)(ZrO_2)_6]$.[5]



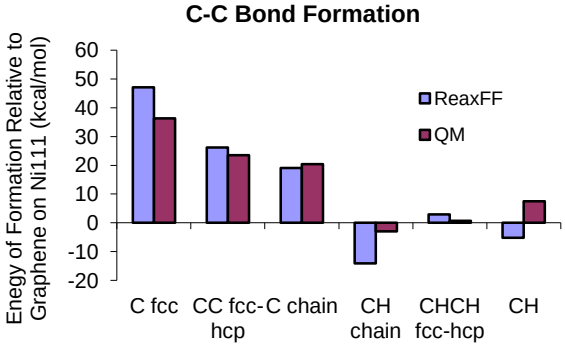
QM- and ReaxFF surface energies for the orthorhombic(space group *Pbca*) ZrO_2 phase.[5]



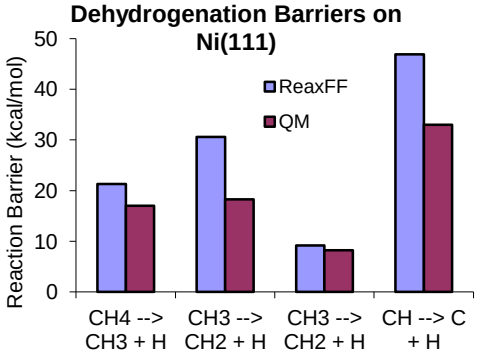
Calculated and experimental YSZ oxygen diffusion coefficients as a function of temperature (top) and 1000/T (bottom).[5]



ReaxFF fit to EOS for various nickel crystal structures.



ReaxFF energy trends in formation of C-C bonds for extended carbon structures.



ReaxFF fit for barriers for methane decomposition on Ni(111).

Table. Comparison of reaction products for n-butane conversion from experiment[17] and ReaxFF MD.

Theory	$8\times C_4H_{10}$	$10\times H_2O$	$2\times CH_4$	$1\times C_2H_4$	$1\times C_2H_6$	$2\times C_3H_6$	$15\times C_n$	$5\times H_2$
Experiment	$n\times C_4H_{10}$	H_2O	CH_4	C_2H_4	C_2H_6	C_3H_6	C_n	H_2