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

Development and Application of ReaxFF Methodology for Understanding the Chemical Dynamics of Metal Carbonates in Aqueous Solutions

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Reactive MD-force field: Protein force field Dec 8 2015 + Pitman
Na/Ca/Mg/C/O/H
 39       ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.5469 !Overcoordination parameter
    1.6725 !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
  -20.0000 !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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    1.7602 !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)
    0.7903 !Valency angle conjugation parameter
  7    ! 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    1.3704   4.0000  12.0000   1.8907   0.1868   0.6388   1.1294
4.0000
      9.8017   2.1260   4.0000  30.0000  79.5548   4.9730   6.0000
0.0000
      1.2022   0.0000 197.2908   8.9856  34.9620  13.5366   0.8563
0.0000
     -2.8983   2.3275   1.0564   4.0000   2.9663   0.0000   0.0000
0.0000
 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  55.1878   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  68.0152   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
 Na   1.7878   1.0000  22.9898   2.6441   0.2588   0.8476  -1.0000
1.0000
      9.0003   2.5000   1.0000   0.0000   0.0000  -3.4731   8.1298
0.0000
     -1.0000   0.0000  23.0445 100.0000   1.0000   0.0000   0.8563
0.0000
     -4.1479   3.9900   1.0338   8.0000   2.5791   0.0010   0.0000
0.0010
 Ca   1.9927   2.0000  40.0870   2.7005   0.1848   0.9605   1.0000
2.0000
     10.6123  27.5993   3.0000  38.0000   0.0000  -1.8731   6.3136
0.0000
     -1.3000   0.0000 220.0000  49.9248   0.3370   0.0000   0.0000
0.0000
```

```
     -2.0000   4.0000   1.0564   6.2998   2.9663   1.4000   0.0100
13.0000
 Mg   1.8330   2.0000  24.3050   2.3591   0.1915   0.5811   1.0000
2.0000
     11.0272   4.4030   3.0000  38.0000   0.0000   1.0577   6.1399
0.0000
     -1.3000   0.0000 127.9160  49.9248   0.3370   0.0000   0.0000
0.0000
     -8.9223   2.3663   1.0564   6.0000   2.9663   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   4.0000   2.8793   0.0000   0.0000
0.0000
 19      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                         pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
  1  1 145.1104  93.6846  57.5621  -0.6831  -0.4472   1.0000  34.9350
0.3881
         0.5276  -0.1073   9.1992   1.0000  -0.0798   6.7209   1.0000
0.0000
  1  2 166.2175   0.0000   0.0000  -0.5944   0.0000   1.0000   6.0000
0.5738
         5.3662   1.0000   0.0000   1.0000  -0.0572   6.9913   0.0000
0.0000
  2  2 153.2532   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
  1  3 157.5526 100.1654  61.2014  -0.5755  -0.3947   1.0000  18.6775
0.4110
         0.9469  -0.4198   7.9115   1.0000  -0.1708   4.9995   0.0000
0.0000
  3  3 142.2858 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
  2  3 160.0000   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  4   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
  2  4  26.7569   0.0000   0.0000   1.0000  -0.3000   1.0000  36.0000
0.0100
         0.5785  -0.3500  25.0000   1.0000  -0.2601   6.6137   1.0000
0.0000
```

```
  3  4  28.0000   0.0000   0.0000   0.4351  -0.3000   1.0000  36.0000
0.0656
        18.6859  -0.3500  25.0000   1.0000  -0.1391   7.4280   1.0000
0.0000
  4  4  72.6003   0.0000   0.0000  -0.7273   0.3000   0.0000  25.0000
0.1919
         6.6441  -0.4000  12.0000   1.0000  -0.0345   5.0063   0.0000
0.0000
  1  5   0.0000   0.0000   0.0000  -0.6528  -0.3000   0.0000  36.0000
0.5000
        10.0663  -0.3500  25.0000   1.0000  -0.1000  10.0000   0.0000
0.0000
  2  5   0.0000   0.0000   0.0000  -0.0203  -0.1418   1.0000  13.1260
0.0230
         8.2136  -0.1310   0.0000   1.0000  -0.2692   6.4254   0.0000
24.4461
  3  5  54.7436   0.0000  44.9919   1.0000  -0.3000   1.0000  36.0000
-0.0346
         0.5457  -0.2500  12.0000   1.0000  -0.0422   8.7778   1.0000
24.4461
  4  5   0.1000   0.0000   0.0000   0.5000  -0.3000   1.0000  16.0000
0.5000
         0.5000  -0.2500  15.0000   1.0000  -0.1000   9.0000   0.0000
0.0000
  5  5  36.9494   0.0000   0.0000  -0.0412  -0.2000   0.0000  16.0000
0.3233
         0.3708  -0.2000  10.0000   1.0000  -0.0822   4.2104   0.0000
0.0000
  1  6   0.0000   0.0000   0.0000  -0.6528  -0.3000   0.0000  36.0000
0.5000
        10.0663  -0.3500  25.0000   1.0000  -0.1000  10.0000   0.0000
0.0000
  2  6  58.6896   0.0000   0.0000  -0.0203  -0.1418   1.0000  13.1260
0.0230
         8.2136  -0.1310   0.0000   1.0000  -0.2692   6.4254   0.0000
24.4461
  3  6  73.0072   0.0000  43.3991   0.8309  -0.3000   1.0000  36.0000
0.2121
         0.5015  -0.2500  12.0000   1.0000  -0.0545   6.7425   1.0000
24.4461
  6  6  40.5111   0.0000   0.0000   0.2563  -0.2000   0.0000  16.0000
0.2232
         1.5087  -0.2000  10.0000   1.0000  -0.1416   4.4975   0.0000
0.0000
 13    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
  1  2   0.1206   1.3998   9.8420   1.1177  -1.0000  -1.0000
  2  3   0.0283   1.2885  10.9190   0.9215  -1.0000  -1.0000
  1  3   0.0672   1.8208  10.0991   1.4000   1.1705   1.0634
  1  4   0.1923   2.4000   9.0446  -1.0000  -1.0000  -1.0000
  2  4   0.1100   1.8410   9.1430   1.7735  -1.0000  -1.0000
  3  4   0.1497   1.5719  13.3058   1.6111  -1.0000  -1.0000
  1  5   0.1752   1.0003  14.0000  -1.0000  -1.0000  -1.0000
```

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  2  5   0.0100   1.6000  13.2979  -1.0000  -1.0000  -1.0000
  3  5   0.1394   1.7472  11.8770   1.9198  -1.0000  -1.0000
  4  5   0.0100   1.4271  10.8031  -1.0000  -1.0000  -1.0000
  1  6   0.4000   1.7604  14.0000  -1.0000  -1.0000  -1.0000
  2  6   0.0100   1.6000  13.2979   1.8670  -1.0000  -1.0000
  3  6   0.0566   1.7000  11.6385   1.5120  -1.0000  -1.0000
 39    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
  1  1  1  67.2380  40.0000   0.9471   0.0000   0.6938  14.9916
1.3673
  1  1  2  66.1046  14.4379   6.0443   0.0000   0.9851   0.0000
2.7063
  2  1  2  68.2534  24.9110   3.7590   0.0000   1.5457   0.0000
2.9366
  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  59.2685  25.8472   1.7572   0.0000   4.4967  58.6562
1.1553
  3  1  3  75.1448  11.4232   5.2677 -14.2010   1.1419   0.0000
2.2364
  2  1  3  59.2133  26.6398   1.1864   0.0000   0.1245   0.0000
1.5701
  1  3  1  57.8946  31.9211   0.7959   0.0000   2.4921   0.0000
1.7123
  1  3  3  83.1701  45.0000   1.5698   0.0000   1.1034  68.1072
1.5349
  3  3  3  87.3324  15.8235   2.7528   0.0000   2.9390   0.0000
1.0000
  1  3  2  90.0000   7.3724   5.3059   0.0000   1.2146   0.0000
3.0000
  2  3  3  75.6935  50.0000   2.0000   0.0000   1.0000   0.0000
1.1680
  2  3  2  85.8000   9.8453   2.2720   0.0000   2.8635   0.0000
1.5800
  1  2  3   0.0000  19.9767   1.1358   0.0000   0.6225   0.0000
1.0432
  3  2  3   0.0000  10.7350   5.0000   0.0000   0.0000   0.0000
4.0000
  2  2  3   0.0000   8.5744   3.0000   0.0000   0.0000   0.0000
1.0421
  3  4  3 100.0000  45.9627   3.0941   0.0000   3.2848   0.0000
2.0000
  2  3  4  87.9313   7.1387   3.0639   0.0000   1.5000   0.0000
1.5554
  4  3  4  84.9984   6.4965   1.5553   0.0000   1.0368   0.0000
2.0000
  3  3  4  70.0000  25.0000   1.0000   0.0000   1.0000   0.0000
1.2500
```

```
  1  3  4  90.0000   3.3724   3.0000   0.0000   0.5224   0.0000
1.1707
  3  5  3   0.2500   2.5141   2.9175   0.0000   0.7479   0.0000
1.5658
  5  3  5   1.0000   1.3180   3.0871   0.0000   1.9285   0.0000
2.2776
  2  3  5  51.3829   2.5000   0.2500   0.0000   0.0500   0.0000
1.0000
  3  3  5  78.9180  19.1144   0.9887   0.0000   1.0012   0.0000
1.2276
  4  3  5 106.3744  30.0000   3.5000   0.0000   2.8611   0.0000
3.0000
  1  3  5  52.5052  24.9776   3.0000   0.0000   2.0000   0.0000
1.5611
  2  6  2   0.0000  49.8261   0.2093   0.0000   2.0870   0.0000
2.2895
  2  2  6   0.0000  40.0366   3.1505   0.0000   1.1296   0.0000
1.1110
  6  2  6   0.0000   0.5047   0.8000   0.0000   0.8933   0.0000
4.6650
  2  6  6   0.0000   8.7037   0.0827   0.0000   3.5597   0.0000
1.1198
  3  6  3   0.0000  14.7597   0.1543   0.0000   1.0000   0.0000
1.0400
  6  3  6  26.2240  12.7492   1.9545   0.0000   1.0000   0.0000
3.0000
  2  3  6  62.5265  13.3742   3.1885   0.0000   1.0000   0.0000
1.6975
  2  6  3   0.0000  35.0000   0.3447   0.0000   1.0000   0.0000
1.9494
  3  3  6  70.0000  20.0000   1.0000   0.0000   1.0000   0.0000
1.2500
  1  3  6  75.7058   4.5836   3.0000   0.0000   0.0500   0.0000
1.9315
 26    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
  1  1  1  1  -0.5000  38.4080   0.5000  -6.1117  -1.9481   0.0000
0.0000
  1  1  1  2   0.4247  27.7539   0.5000  -6.3112  -1.9452   0.0000
0.0000
  2  1  1  2  -0.5000  30.7919   0.5000  -5.8539  -3.0000   0.0000
0.0000
  1  1  1  3  -0.1108  80.0000  -0.5793  -5.4405  -1.1000   0.0000
0.0000
  2  1  1  3  -0.5732  28.8617   0.8920  -5.1112  -1.0978   0.0000
0.0000
  3  1  1  3  -1.7931  25.6020  -1.0000  -4.0381  -0.8614   0.0000
0.0000
  1  1  3  1   1.0000  59.3911  -0.5000  -2.7048  -0.9000   0.0000
0.0000
  1  1  3  2  -0.1141   5.0000  -1.0000  -8.1021  -0.9000   0.0000
0.0000
```

```
  2  1  3  1   2.5000  15.2653   0.8965  -2.5000  -0.9000   0.0000
0.0000
  2  1  3  2  -2.5000  37.1322   0.4144  -4.6988  -1.1000   0.0000
0.0000
  2  1  3  3   0.8151 100.0000   1.0000  -3.4409  -2.8274   0.0000
0.0000
  3  1  3  1   0.5406  16.8262   0.4979  -8.2524  -3.0437   0.0000
0.0000
  3  1  3  2   2.4679  16.0446  -0.3246  -2.5000  -3.0476   0.0000
0.0000
  1  3  3  2  -2.5000   7.3697  -1.0000  -4.1837  -2.9498   0.0000
0.0000
  2  3  3  2  -2.5000 -25.0000  -1.0000  -2.5000   0.0000   0.0000
0.0000
  1  3  3  3   2.5000 -24.1204   1.0000  -3.2189  -0.9972   0.0000
0.0000
  2  3  3  3  -2.0407  80.0000  -0.9677  -7.0890   0.0000   0.0000
0.0000
  3  3  3  3  -2.5000 -25.0000   1.0000  -2.5000  -0.9000   0.0000
0.0000
  0  1  2  0   2.0735   0.1000   0.0100  -4.0000   0.0000   0.0000
0.0000
  0  2  2  0   0.0000   0.1000   0.0100  -4.0000   0.0000   0.0000
0.0000
  0  2  3  0   0.0000   0.1000   0.0200  -4.0000   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
  1  1  3  3  -0.0002  20.1851   0.1601  -9.0000  -2.0000   0.0000
0.0000
  1  3  3  1   0.0002  80.0000  -1.5000  -4.4848  -2.0000   0.0000
0.0000
  3  1  3  3  -0.1583  20.0000   1.5000  -9.0000  -2.0000   0.0000
0.0000
  1    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
  3  2  3   2.1200  -3.5800   1.4500  19.5000
```