Supplementary Information

Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers

Aniruddh Vashisth*, Chowdhury Ashraf[#], Weiwei Zhang[#], Charles E. Bakis* and Adri C.T. van Duin*[#]

*Department of Engineering Science and Mechanics, The Pennsylvania State University, 212 Earth and Engineering Sciences Building, University Park, Pennsylvania, 16802
[#] Department of Mechanical Engineering, The Pennsylvania State University, 136 Research East Building, Bigler Road, University Park, Pennsylvania, 16802

ReaxFF Force Field

As mentioned in the manuscript, the re-optimization force field based on the parameters of CHNO-2017_weak [1] are given below. For all the examinations carried out in this study, the force field defined by these parameters was used.

```
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)
   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
11    ! 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    1.3727   4.0000  12.0000   2.0270   0.1113   0.5516   1.1706   4.0000
     9.2293   4.5389   4.0000  30.0000  79.5548   4.4087   7.0601   0.0000
     1.1168   0.0000 181.0000  14.5210  24.9431   6.7313   0.8563   0.0000
    -6.7437   5.6329   1.0564   4.0000   2.9663   0.0000   0.0000   0.0000
H    0.8924   1.0000   1.0080   1.6791   0.0709   0.7390  -0.1000   1.0000
     8.3519  39.1732   1.0000   0.0000 121.1250   3.5442   9.3848   1.0000
    -0.1000   0.0000  61.6606   2.8222   2.1441   0.0003   1.0698   0.0000
   -18.1423   5.3143   1.0338   1.0000   2.8793   0.0000   0.0000   0.0000
O    1.2450   2.0000  15.9990   2.3396   0.1000   1.1000   1.0548   6.0000
     9.3187  12.5083   4.0000  37.5000 116.0768   8.5000   8.4783   2.0000
     0.9049   0.1000  59.0626   3.4340   0.7722   0.0021   0.9745   0.0000
    -3.5352   3.2703   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
N    1.2333   3.0000  14.0000   1.9690   0.1513   1.0000   1.1748   5.0000
     9.6326   9.1048   4.0000  32.4838 100.0000   6.6335   7.1473   2.0000
     1.0433   2.3175 119.9837   0.4648   9.7074   2.2521   0.9745   0.0000
    -7.0000   4.0000   1.0183   4.0000   2.8793   0.0000   0.0000   0.0000
S    1.9673   2.0000  32.0600   2.1729   0.3000   1.0336   1.5359   6.0000
    10.3008   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
   -11.0000   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
Mg   1.8315   2.0000  24.3050   2.2464   0.1806   0.5020   1.0000   2.0000
    10.9186  27.1205   3.0000  38.0000   0.0000   0.9499   5.6130   0.0000
    -1.3000   0.0000 220.0000  49.9248   0.3370   0.0000   0.0000   0.0000
    -1.0823   2.3663   1.0564   6.0000   2.9663   0.0000   0.0000   0.0000
P    1.5994   3.0000  30.9738   1.7000   0.1743   1.0000   1.3000   5.0000
     9.1909  12.0377   5.0000   0.0000   0.0000   1.7681   6.9748   0.0000
    -1.0000  13.1397 125.6300   0.2526  16.9194  24.7770   0.0000   0.0000
    -9.7896   3.3929   1.0338   5.0000   2.8793   0.0000   0.0000   0.0000
Na   2.0300   1.0000  22.9898   2.3334   0.1481   0.8765  -1.0000   1.0000
    11.0000   9.8000   1.0000   0.0000   0.0000  -3.8501   5.9459   0.0000
    -1.0000   0.0000  67.5458 100.0000  10.0000   0.2500   0.8563   0.0000
    -2.5766   2.5000   1.0338   6.0000   2.5791   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
 43      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                        pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
  1  1  91.8588 120.2415  50.6788   0.3723  -0.1000   1.0000  34.6637
0.7015
         6.8558  -0.1605   7.9139   1.0000  -0.0719   6.9788   1.0000
0.0000
  1  2 185.0817   0.0000   0.0000  -0.4949   0.0000   1.0000   6.0000
0.6864
         8.2839   1.0000   0.0000   1.0000  -0.0847   6.4150   0.0000
0.0000
  2  2 165.6186   0.0000   0.0000  -0.4194   0.0000   1.0000   6.0000
0.6197
         6.3245   1.0000   0.0000   1.0000  -0.0879   6.0634   0.0000
0.0000
  1  3 148.9918 115.2723  93.5449  -0.6834  -0.3639   1.0000  18.9178
0.6790
         0.4084  -0.4385   7.7418   1.0000  -0.1798   4.9342   0.0000
0.0000
  2  3 159.4722   0.0000   0.0000  -0.5725   0.0000   1.0000   6.0000
0.5505
         1.1150   1.0000   0.0000   0.0000  -0.0920   4.2790   0.0000
0.0000
  3  3 142.2858  85.0000   0.0000   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  4 186.9647  90.5539  69.0633  -1.7565  -0.1960   1.0000  28.5338
0.1967
         0.0446  -0.3644   6.5414   1.0000  -0.2803   4.6293   1.0000
0.0000
  3  4 128.8596 167.8643  40.0000   0.3819  -0.1539   1.0000  34.9972
0.1900
         1.0110  -0.3716   7.0805   1.0000  -0.1265   6.8843   1.0000
0.0000
  4  4 160.1592  82.5526 153.9884   0.4110  -0.0934   1.0000  12.4304
0.5899
         0.1538  -0.1473  11.9187   1.0000  -0.0753   5.4371   1.0000
0.0000
  2  4 173.4757   0.0000   0.0000  -0.2904   0.0000   1.0000   6.0000
0.6709
```

```
         0.5347   1.0000   0.0000   1.0000  -0.1855   5.2649   0.0000
0.0000
  1   5 150.8132  59.3363  55.2528  -0.0628  -0.5211   1.0000  18.9617
0.3219
         0.3317  -0.2289   7.5946   1.0000  -0.1946   5.9455   1.0000
0.0000
  2   5 143.4377   0.0000   0.0000  -0.2944   0.0000   1.0000   6.0000
0.6034
         9.5627   1.0000   0.0000   1.0000  -0.0516   7.0960   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
  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   5 140.8887  84.9350  68.6860  -0.4111  -0.4781   1.0000  17.8574  -
0.1336
         0.2881  -0.2494   9.8436   1.0000  -0.1806   7.4732   1.0000
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  87.0227   0.0000  43.3991   0.0030  -0.3000   1.0000  36.0000
0.0250
         0.0087  -0.2500  12.0000   1.0000  -0.0439   6.6073   1.0000
24.4461
  6   6  32.3808   0.0000   0.0000  -0.0076  -0.2000   0.0000  16.0000
0.2641
         4.8726  -0.2000  10.0000   1.0000  -0.0729   4.6319   0.0000
0.0000
  1   7   0.0000   0.0000   0.0000   0.2171  -0.1418   1.0000  13.1260
0.6000
         0.3601  -0.2500  20.0000   1.0000  -0.2000  10.0000   1.0000
0.0000
  2   7   0.0000   0.0000   0.0000   0.2250  -0.1418   1.0000  13.1260
0.6000
         0.3912  -0.1310   0.0000   1.0000  -0.2000  10.0000   0.0000
0.0000
  3   7 250.0000 182.8454   0.0000   0.0607  -0.5000   1.0000  25.0000
0.4547
         0.7012  -0.2197  15.9047   1.0000  -0.2026   6.4270   1.0000
0.0000
  4   7 130.0000   0.0000   0.0000   0.2171  -0.1418   1.0000  13.1260
0.6000
         0.3601  -0.1310  10.7257   1.0000  -0.0869   5.3302   1.0000
0.0000
```

```
  6  7   0.1000   0.0000   0.0000   0.2500  -0.5000   1.0000  35.0000
0.6000
        0.5000  -0.5000  20.0000   1.0000  -0.2000  10.0000   1.0000
0.0000
  7  7   0.0000   0.0000   0.0000   0.2171  -0.5000   1.0000  35.0000
0.6000
        0.5000  -0.5000  20.0000   1.0000  -0.2000  10.0000   1.0000
0.0000
  2  8   0.0000   0.0000   0.0000  -1.0000  -0.3000   1.0000  36.0000
0.7000
       10.1151  -0.3500  25.0000   1.0000  -0.1053   8.2003   1.0000
0.0000
  3  8  76.0753   0.0000   0.0000  -0.4452  -0.3000   1.0000  36.0000
0.6433
        5.6834  -0.3500  25.0000   1.0000  -0.0539   8.0273   1.0000
0.0000
  4  8   0.0000   0.0000   0.0000  -1.0000  -0.3000   1.0000  36.0000
0.7000
       10.1151  -0.3500  25.0000   1.0000  -0.1053   8.2003   1.0000
0.0000
  6  8   0.1000   0.0000   0.0000   0.2500  -0.5000   1.0000  35.0000
0.6000
        0.5000  -0.5000  20.0000   1.0000  -0.2000  10.0000   1.0000
0.0000
  7  8   0.1000   0.0000   0.0000   0.2500  -0.5000   1.0000  35.0000
0.6000
        0.5000  -0.5000  20.0000   1.0000  -0.2000  10.0000   1.0000
0.0000
  8  8  27.8052   0.0000   0.0000   0.4022   0.3000   0.0000  25.0000
0.4894
        0.6222  -0.4000  12.0000   1.0000  -0.0500   5.3362   0.0000
0.0000
  4  6   0.0000   0.0000   0.0000  -1.0000  -0.3000   1.0000  36.0000
0.7000
       10.1151  -0.3500  25.0000   1.0000  -0.1053   8.2003   1.0000
0.0000
  1  9   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  9   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
  3  9  81.4346   0.0000   0.0000  -0.1594  -0.3000   1.0000  36.0000
0.0025
        0.2904  -0.2500  12.0000   1.0000  -0.0742   9.3638   0.0000
0.0000
  4  9  96.5322   0.0000   0.0000   0.9970  -0.3000   1.0000  36.0000
0.5095
```

```
         0.7247  -0.2500  12.0000   1.0000  -0.1175   9.9985   0.0000
0.0000
  9  9  73.6263   0.0000   0.0000   0.0209  -0.2000   0.0000  16.0000
0.3414
         0.4703  -0.2000  15.0000   1.0000  -0.1319   5.9254   0.0000
0.0000
  2 10 109.1686   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
  3 10   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
  9 10 118.3052   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
 10 10   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
  1  8   0.0000   0.0000   0.0000  -1.0000  -0.3000   1.0000  36.0000
0.7000
        10.1151  -0.3500  25.0000   1.0000  -0.1053   8.2003   1.0000
0.0000
  1 10   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
  4 10   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
 24    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
  1  2   0.1163   1.3831   9.9402   1.1471  -1.0000  -1.0000
  1  3   0.0729   2.0641   9.6888   1.4359   1.1638   1.0702
  2  3   0.0283   1.2853  10.9173   0.9259  -1.0000  -1.0000
  1  4   0.1268   1.9685   9.7237   1.3409   1.2578   1.1715
  2  4   0.1140   1.4837   9.0464   1.0812  -1.0000  -1.0000
  3  4   0.2000   1.8111   9.3860   1.4308   1.0787   1.2599
  1  5   0.1618   1.7943  10.1042   1.7489   1.3150   1.4031
  2  5   0.0764   1.5838  10.1462   1.4206  -1.0000  -1.0000
  3  5   0.1022   1.9887  10.0605   1.5799   1.4000  -1.0000
  4  5   0.1505   1.9000  10.5104   1.8000   1.4000  -1.0000
  2  6   0.0100   1.6000  13.2979   1.8670  -1.0000  -1.0000
  3  6   0.0809   1.7000  11.4606   1.5177  -1.0000  -1.0000
  1  7   0.2291   1.7500  10.0393  -1.0000  -1.0000  -1.0000
  2  7   0.3000   1.9262  10.0302  -1.0000  -1.0000  -1.0000
  3  7   0.1573   1.8644  10.1395   1.7435   1.4412  -1.0000
```

```
  6  7   0.1801   1.8566   9.8498   0.1000  -1.0000  -1.0000
  3  8   0.1592   1.8283  11.7256   1.6655  -1.0000  -1.0000
  1  9   0.0500   1.7500  12.3500   0.1000  -1.0000  -1.0000
  2  9   0.0300   1.5200  12.5000   0.1000  -1.0000  -1.0000
  3  9   0.0348   1.7637  12.3562   1.7228  -1.0000  -1.0000
  4  9   0.0478   1.7704  12.8051   1.6100  -1.0000  -1.0000
  2 10   0.0568   1.6740   9.6297   1.2200  -1.0000  -1.0000
  3 10   0.1927   2.2551  11.2308  -1.0000  -1.0000  -1.0000
  9 10   0.1402   2.1604  10.9786   1.7505  -1.0000  -1.0000
105    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
  1  1  1  66.0347  45.0000   1.1248   0.0000   3.0000  70.0000   2.4142
  1  1  2  58.9292  15.1099   4.4631   0.0000   0.0287   0.0000   1.8837
  2  1  2  64.8992  17.4932   1.9470   0.0000   3.0000   0.0000   1.0135
  1  2  2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000   1.0400
  1  2  1   0.0000   7.5000   5.0000   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  51.7494  42.2658   0.7914   0.0000   4.0000  58.6562   1.7461
  3  1  3  72.7766   9.2311   7.5000 -20.0000   1.1419   0.0000   1.4603
  1  1  4  58.4756  41.7584   0.6211   0.0000   1.4838   0.0000   1.6722
  3  1  4  79.3051  13.4668   1.9350   0.0000   0.4036  32.5000   1.3503
  4  1  4  65.2722   4.5000   0.4741   0.0000   0.9683   0.0000   2.1819
  2  1  3  59.1567  27.4483   1.1736   0.0000   0.1000   0.0000   1.6111
  2  1  4  61.4983  11.5971   2.1170   0.0000   0.1000   0.0000   1.2079
  1  2  4   0.0000   0.0019   6.3000   0.0000   0.0000   0.0000   1.0400
  1  3  1  68.7170   6.5547   0.5383   0.0000   2.2753   0.0000   1.8466
  1  3  3  82.6613  45.0000   1.3380   0.0000   1.1034  68.1072   1.6232
  1  3  4  90.0000  18.7269   1.4975   0.0000   3.0479   0.0000   1.0965
  3  3  3  90.0000  25.0984   1.6910   0.0000   1.6310  50.0000   1.0000
  3  3  4  82.4170  34.0230   1.0276   0.0000   2.6572   0.0000   1.4288
  4  3  4  72.6356  45.0000   1.1114   0.0000   3.0072   0.0000   1.0000
  1  3  2  90.0000   8.9828   2.3727   0.0000   1.2146   0.0000   3.0000
  2  3  3  79.5453  50.0000   2.1630   0.0000   3.0000   0.0000   1.2391
  2  3  4  69.4868  16.3078   4.4440   0.0000   0.2502   0.0000   1.8860
  2  3  2  85.7876   9.3298   2.0747   0.0000   2.8632   0.0000   1.6905
  1  4  1  81.6738  11.0200   1.6084   0.0000   2.7249   0.0000   1.4096
  1  4  3  88.8926   9.1088   4.8453   0.0000   2.1900   0.0000   3.0000
  1  4  4  71.4079  13.7291   2.6469   0.0000   2.9290   0.0000   3.0000
  3  4  3  74.7164  43.0000   1.1816 -18.0069   3.0584   0.0000   1.1322
  3  4  4  81.1388  40.7000   0.9549  -0.9193   3.0760   0.0000   1.0000
  4  4  4  72.1841  29.8125   1.9658   0.0000   2.9239   0.0000   2.9000
  1  4  2  88.7155   6.5761   1.8952   0.0000   0.2894   0.0000   1.1321
  2  4  3  76.0014  10.1041   7.3108   0.0000   0.4346   0.0000   3.0000
  2  4  4  90.0000  42.7711   1.4427   0.0000   0.1000   0.0000   1.1775
  2  4  2  83.5503  12.3251   4.8243   0.0000   0.1777   0.0000   1.0020
  1  2  3   0.0000  17.0624   0.9927   0.0000   0.6225   0.0000   1.0000
  1  2  4   0.0000  19.3874   0.2427   0.0000   0.2078   0.0000   1.1303
  1  2  5   0.0000  15.0000   3.0000   0.0000   0.0000   0.0000   1.0400
  3  2  3   0.0000   1.0000   2.5054   0.0000   0.0000   0.0000   4.0000
  3  2  4   0.0000  12.4279   2.9774   0.0000   0.1224   0.0000   1.8030
  4  2  4   0.0000  20.0000   3.6106   0.0000   0.1460   0.0000   1.0000
```

2	2	3	0.0000	5.8938	3.0000	0.0000	0.0000	0.0000	1.0629
2	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	1	5	74.4180	33.4273	1.7018	0.1463	0.5000	0.0000	1.6178
1	5	1	79.7037	28.2036	1.7073	0.1463	0.5000	0.0000	1.6453
2	1	5	63.3289	29.4225	2.1326	0.0000	0.5000	0.0000	3.0000
1	5	2	85.9449	38.3109	1.2492	0.0000	0.5000	0.0000	1.1000
1	5	5	80.0000	25.0000	2.0000	0.0000	0.5000	0.0000	1.3830
2	5	2	85.0000	15.1317	2.0000	0.0000	0.5000	0.0000	2.0000
2	5	5	97.0064	32.1121	2.0242	0.0000	0.5000	0.0000	2.8568
2	2	5	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
5	4	5	62.0000	33.4273	1.7018	0.1463	0.5000	0.0000	1.0500
3	5	3	77.0699	39.4349	2.1313	-30.0000	0.9567	0.0000	1.1483
1	5	3	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
1	5	4	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
4	1	5	60.0000	35.0000	3.0223	0.0000	2.3550	0.0000	1.2002
3	5	4	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
5	1	7	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
1	3	5	73.0990	33.8942	1.2098	0.0000	0.8161	0.0000	1.1776
3	3	5	83.9753	31.0715	3.5590	0.0000	0.8161	0.0000	1.1776
2	3	5	76.9521	20.0000	2.0903	0.0000	1.0000	0.0000	1.0400
2	6	2	0.0000	49.8261	0.2093	0.0000	2.0870	0.0000	2.2895
2	2	6	0.0000	39.7818	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	9.2317	0.1000	0.0000	1.0000	0.0000	1.0920
6	3	6	0.0008	25.0000	8.0000	0.0000	1.0000	0.0000	3.0000
2	3	6	66.0423	5.0000	1.0000	0.0000	1.0000	0.0000	1.2500
2	6	3	0.0000	0.5000	0.1000	0.0000	1.0000	0.0000	3.0000
3	3	6	70.0000	20.0000	1.0000	0.0000	1.0000	0.0000	1.2500
3	7	3	90.0000	6.2396	1.3578	-24.9000	1.5156	0.0000	1.6302
2	3	7	100.0000	11.5040	1.5163	0.0000	3.6982	0.0000	1.0400
3	3	7	60.0000	40.0000	4.0000	0.0000	1.0000	0.0000	1.0400
3	2	7	0.0000	10.0000	1.0000	0.0000	1.0000	0.0000	1.0400
6	3	7	41.7961	3.4184	7.4578	0.0000	-0.2958	0.0000	1.0542
7	3	7	90.0000	16.5250	7.0313	0.0000	-0.0396	0.0000	3.0000
1	3	7	56.0610	4.2889	4.5235	0.0000	2.6593	0.0000	2.4280
2	7	3	75.0000	25.0000	2.0000	0.0000	1.0000	0.0000	1.2500
3	7	7	70.0000	25.0000	2.0000	0.0000	1.0000	0.0000	1.2500
3	9	3	96.2265	4.5610	12.0000	0.0000	0.3211	0.0000	1.5204
3	9	3	0.0000	9.1552	7.9919	0.0000	0.1660	0.0000	1.5386
9	3	9	100.0000	10.1065	6.0000	0.0000	1.0000	0.0000	3.6601
2	3	9	55.0417	3.5032	3.9979	0.0000	1.5171	0.0000	1.0400
3	3	9	70.0000	30.0000	2.0000	0.0000	1.0000	0.0000	1.2500
3	9	9	66.7783	14.3146	0.7911	0.0000	1.0000	0.0000	1.2333
3	9	10	96.6924	9.4823	5.7883	0.0000	0.2248	0.0000	2.2640
3	9	10	0.0000	3.8549	3.7230	0.0000	0.1482	0.0000	1.0400
9	10	9	0.0000	11.2336	6.8851	0.0000	1.0000	0.0000	1.0893
9	9	10	90.0000	5.0811	5.2147	0.0000	1.0000	0.0000	1.8538
10	9	10	0.0100	21.1482	0.3506	0.0000	1.0000	0.0000	1.4361
3	2	10	0.0000	0.0100	0.5211	0.0000	0.0000	0.0000	1.3859

```
 3  9  4 100.0000  28.1532  12.0000   0.0000   0.2932   0.0000   1.6489
 3  9  4   0.0000  22.7457   2.9039   0.0000   0.5593   0.0000   1.9764
 4  9  4  87.0081  27.6432   3.9735   0.0000   4.0000   0.0000   1.4578
 4  9  4   0.0000  22.8998   3.1077   0.0000   3.0000   0.0000   1.0696
 9  4  9 100.0000  10.1065   6.0000   0.0000   1.0000   0.0000   3.6601
 2  4  9  80.0000   3.5601   3.3645   0.0000   1.5171   0.0000   1.0400
 3  4  9  70.0000  30.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 4  3  9  70.0000  30.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 4  4  9  70.0000  30.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 4  9  9  66.7783  14.3146   0.7911   0.0000   1.0000   0.0000   1.2333
 4  9 10  95.2122   5.7090  12.0000   0.0000   0.2248   0.0000   2.8936
 4  9 10   0.0000   9.0054   7.9511   0.0000   0.1482   0.0000   1.6245
 4  2 10   0.0000  15.0000   2.8900   0.0000   0.0000   0.0000   2.8774
 1  3  9  55.0000  15.0000   1.0000   0.0000   1.0000   0.0000   1.5000
 1  4  9  55.0000  15.0000   1.0000   0.0000   1.0000   0.0000   1.5000
66    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1  1  1  1   0.3619   5.0000   0.2257  -9.0000  -2.4400   0.0000   0.0000
 1  1  1  2   0.2330  56.0330  -0.0369  -6.3749  -1.6179   0.0000   0.0000
 2  1  1  2  -0.0662  44.7480   0.3945  -6.5879  -3.0000   0.0000   0.0000
 1  1  1  3   2.0835  80.0000   0.2861  -5.8354  -1.1000   0.0000   0.0000
 2  1  1  3   2.5000  15.1318   1.0000  -6.3682  -1.0978   0.0000   0.0000
 3  1  1  3  -1.4902  25.2456  -1.0000  -2.5000  -0.8614   0.0000   0.0000
 1  1  3  1  -1.0000  -5.0000  -0.5000  -2.5000  -0.9000   0.0000   0.0000
 1  1  3  2  -2.1885   5.0000  -0.9943  -9.0000  -0.9000   0.0000   0.0000
 2  1  3  1   0.8086  63.4490  -0.1261  -9.0000  -0.9000   0.0000   0.0000
 2  1  3  2  -2.5000  73.5049   0.8863  -4.0386  -1.1000   0.0000   0.0000
 2  1  3  3  -0.9280 100.0000   1.0000  -3.9313  -2.8274   0.0000   0.0000
 3  1  3  1  -2.5000   9.3090  -1.0000  -8.2407  -3.0437   0.0000   0.0000
 3  1  3  2   2.5000  21.4615  -0.0315  -2.5000  -3.0476   0.0000   0.0000
 1  3  3  2  -2.5000   8.2305  -0.2363  -2.7513  -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   1.5042 -24.6836   1.0000  -2.5000  -0.9972   0.0000   0.0000
 2  3  3  3   0.2942  70.1282  -0.7126  -6.1638   0.0000   0.0000   0.0000
 3  3  3  3  -2.5000 -25.0000   1.0000  -2.5000  -0.9000   0.0000   0.0000
 1  1  4  2   0.7954  67.9069   0.3504  -8.0000  -1.9825   0.0000   0.0000
 2  1  4  2   0.4566  46.1133   0.4807  -5.7278  -2.1051   0.0000   0.0000
 3  1  4  2   1.0000  26.3717   1.0000  -3.5214  -2.5261   0.0000   0.0000
 3  1  1  4  -0.5802   7.2544   1.0000  -2.5000  -0.9511   0.0000   0.0000
 4  1  1  4  -0.2416  15.8213  -0.5000  -3.2327  -1.7241   0.0000   0.0000
 1  1  4  1  -1.0000  51.5166   0.1228  -6.5755  -1.6589   0.0000   0.0000
 3  1  4  1  -1.0000  14.9858   1.0000  -8.0000  -1.8038   0.0000   0.0000
 2  1  1  4   1.0000   0.0100   0.8120  -2.8086  -1.9000   0.0000   0.0000
 4  1  4  2   1.0000  51.6090  -0.5000  -3.9390  -2.0202   0.0000   0.0000
 2  1  4  1  -0.2342  68.6969   0.1904  -5.3454  -0.0100   0.0000   0.0000
 4  1  3  1  -0.8484  15.6632  -0.3865  -2.5000  -3.0437   0.0000   0.0000
 4  1  3  2   0.0107   3.7120  -0.5000  -7.9280  -3.0476   0.0000   0.0000
 1  1  1  4   0.9187  -5.0000   1.0000  -6.3298  -2.0000   0.0000   0.0000
 4  1  4  1  -0.8232  16.3430   0.5477  -7.0692  -2.0051   0.0000   0.0000
 0  1  2  0   0.0000   0.0000   0.0000  -4.0000   0.0000   0.0000   0.0000
 0  2  2  0   0.0000   0.0000   0.0000  -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
0  1  4  0   0.2176  40.4126   0.3535  -3.9875  -2.0051   0.0000   0.0000
0  2  4  0   0.0000   0.1000   0.0100  -5.0000   0.0000   0.0000   0.0000
0  3  4  0   1.1397  61.3225   0.5139  -3.8507  -2.7831   0.0000   0.0000
0  4  4  0   0.7265  44.3155   1.0000  -4.4046  -2.0000   0.0000   0.0000
4  1  4  4  -0.0949   8.7582   0.3310  -7.9430  -2.0000   0.0000   0.0000
0  1  5  0   0.8251  92.1468   0.7176  -4.2341   0.0000   0.0000   0.0000
0  5  5  0   0.1291  -5.0000   0.9649  -5.0903   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
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
2  3  9  3  -1.5000   6.8333  -0.1978  -1.4683   0.0000   0.0000   0.0000
2  3  9  4  -0.6181   7.1542  -0.0047  -1.6577   0.0000   0.0000   0.0000
2  4  9  3  -1.5000   1.7820  -1.0000  -5.4916   0.0000   0.0000   0.0000
2  4  9  4  -0.1959   2.3626  -1.0000  -3.0702   0.0000   0.0000   0.0000
2  1  4  9   0.0000  10.0000   0.3000  -6.0000  -1.0000   0.0000   0.0000
2  3  9 10   0.1589  12.5000   0.4388  -1.5000   0.0000   0.0000   0.0000
7  1  1  7   1.0657  78.7067   0.6978  -8.4833  -1.7255   0.0000   0.0000
0  1  7  0   1.4891  35.1275   0.8254  -2.8518   0.0000   0.0000   0.0000
0  7  7  0  -0.3570  38.0764   0.1676  -6.7257   0.0000   0.0000   0.0000
1  1  1  7  -0.1661  19.8637   0.2351 -10.8000  -1.7255   0.0000   0.0000
2  1  3  7  -1.5000  99.6206   0.0516  -8.1129   0.0000   0.0000   0.0000
2  3  7  3  -1.5000  -1.0000   0.2523  -2.7183   0.0000   0.0000   0.0000
1  3  7  3  -1.5000  50.2166   0.9871  -3.6395   0.0000   0.0000   0.0000
7  3  7  3   1.5000  -0.9128   0.0100  -6.2667   0.0000   0.0000   0.0000
1  1  3  7   0.0000   0.1000   0.0100  -4.0000   0.0000   0.0000   0.0000
9    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
3  2  3   2.1493  -3.8387   1.5230  28.0017
3  2  4   2.0543  -6.3062   1.4500  19.5000
4  2  3   1.7500  -1.8134   1.4500  19.5000
4  2  4   1.8886  -1.8024   1.4500  19.5000
3  2  5   1.5000  -2.0000   1.4500  19.5000
4  2  5   1.5000  -2.0000   1.4500  19.5000
5  2  3   1.5000  -2.0000   1.4500  19.5000
5  2  4   1.5000  -2.0000   1.4500  19.5000
5  2  5   1.5000  -2.0000   1.4500  19.5000
```

Tracking Successful Reactions

The successful or the unsuccessful attempts are reported by "molfra.out" file, which is one of the output files generated by ReaxFF. Also, the energy provided to the system is a function of desired target distances (R_{12}) between atoms from the reactive sites (as shown in Equation 2). Another ReaxFF output file – fort.76 – logs the instantaneous distances between pairs of targeted atoms (R_{ij}). Using R_{12} and R_{ij} and Equation 2, the energy input to the molecule can be calculated. Using molfra.out and fort.76, a successful or an unsuccessful attempt can be monitored. For a successful attempt, the molfra.out reports a new molecule at the end of an accelerated boost (10,000 time-steps in this investigation) provided to the system. If the number of species remain same or the molecular weight of the species remains same after an accelerated boost, the reaction attempt is deemed unsuccessful. Figure 8 presents the accelerated boost energies provided to the system as a function of time (from fort.76). For each corresponding peak in the Figure 8, the successful and the unsuccessful attempts are monitored in the molfra.out file. Therefore Figure 8 is a combined interpretation of molfra.out and fort.76. The extra energy goes to the thermostat in case it is an unsuccessful accelerated simulation.

Force Parameters (F_1, F_2 and R_{12})

Table S1 tabulates different force parameters evaluated for non-catalyzed reaction and ΔE denotes the reaction barrier for each individual case. This barrier energy is an approximate barrier energy, and a precise barrier energy is calculated by carrying out a more sophisticated search using an in-house python code. Usually, the transition state (TS) structure found using this crude method has multiple negative frequencies, therefore is not an accurate representation of the saddle point in potential energy landscape. The python code moves all the atoms of the TS structure in the direction of the eigen vectors for the second negative frequency, doing this repeatedly systematically reduces the negative frequencies except the first one. Therefore, after

the search, a structure which has only one high negative frequency is generated, which is a much closer representation of the saddle point. Additionally, as the predicted TS structure moves closer to the actual TS structure, the energy of the predicted structure also reduces during this process giving a better estimation of the barrier energy in ReaxFF, which is actually reported in Figure 6 and 7. The interested readers are encouraged to contact the authors to have an access to the python code. Since this fine tuning is not possible in actual MD simulation, different combinations of the force parameters were tested, and the combination that gives the energy barrier closest to the actual ReaxFF barrier reported in Figure 6 were used during MD simulation. We highlight (bold and #2) these force parameters that were used in this study in Table S1.

Table S1: Force parameters examined for non-catalyzed reaction between epoxide and ammonia. Units for F_1 are kcal/mol and for F_2 are Å^{-2}.

#	**O – C (1.95 A)**		**O – H (1.1 A)**		**C – N (1.5 A)**		**ΔE (kcal/mol)**
	F_1	F_2	F_1	F_2	F_1	F_2	
1	100	0.3	300	0.75	300	0.75	68.69
2	**50**	**0.5**	**250**	**0.75**	**300**	**0.75**	**61.96**
3	50	0.5	300	1.00	250	0.75	69.83
4	100	0.6	250	1.00	275	0.85	75.31

These selected force parameters are then put in the '*tracking.in*' input file to activate the desired tracing sub-routine in ReaxFF. An example of the '*tracking.in*' file is given below with required explanations.

Tracking Subroutine: "Tracking.in"

```
#Distance regimes
#T at1 at2  mindist maxdist
4   N   C   3.0     8.0     C  O  1.3  1.60  O  H  1.5  8.0  H  N  0.9   1.2
#Restraint settings
#iter nr. at1 at2  target  k1  k2
10000  3  2  3   1.95  50  0.5  3  4  1.1  250  0.75  2  1  1.5  300  0.75
```

The third line in the "tracking.in" file is read by ReaxFF. It first describes the number of atoms that need to be tracked (four in this case). The first pair is N atom and C atom, if these two atoms are within a distance range of 3.0–8.0 Å, then the subroutine moves to the next condition. In the next condition it looks at C (same carbon atom that was tracked in the previous pair) and O atoms and checks if these are within 1.30–1.60 Å range, and so on and so forth. At the end, the subroutine cross-checks that the nitrogen from the first pair (N and C) of atoms is the same as the nitrogen from the last pair of atoms (H and N), tracked by the "tracking.in" subroutine. Once these target distances are satisfied, ReaxFF assigns atom numbers 1,2 3 and 4 to N, C, O and H. This number assignment is similar to the order of tracking that the subroutine followed for each atom. Next the subroutine reads the 6^{th} line that specifies the number of steps for the accelerated boost and the force parameters assigned for each pair of atoms. The first number in line 6 is the number of time steps that each boost is provided (10,000 in this case). The next number is the number of constraints that are being assigned. The next two numbers 2 and 3 specify atom number 2 and 3 which are C and O in this case. Next three numbers are R_{12}, F_1 and F_2 respectively for atom number 2 and 3. The next consecutive sets of five numbers define the constraints for O and H atom pair, and N and H atom pair.

References

(1) Zhang, W.; van Duin, A. C. T. Improvement of the ReaxFF Description for Functionalized Hydrocarbon/Water Weak Interactions in the Condensed Phase. *J. Phys. Chem. B* **2018**, acs.jpcb.8b01127.