Supporting Information (SI)

Improved Description of a Coordinate Bond in the ReaxFF Reactive Force Field

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S1. Parameter Optimization of ReaxFF$_{coord}$

The ReaxFF$_{coord}$ force field for the Fe/C/O system was developed based on the previous ReaxFF reported by Zou et al.[S1,S2], and the ReaxFF$_{coord}$ for C/H/B/N systems was developed based on the previous ReaxFF reported by Pai et al.[S3]. For parameter optimization, a modified metropolis Monte Carlo (MMC) algorithm based on the work of Iype et al.[S4] was used.

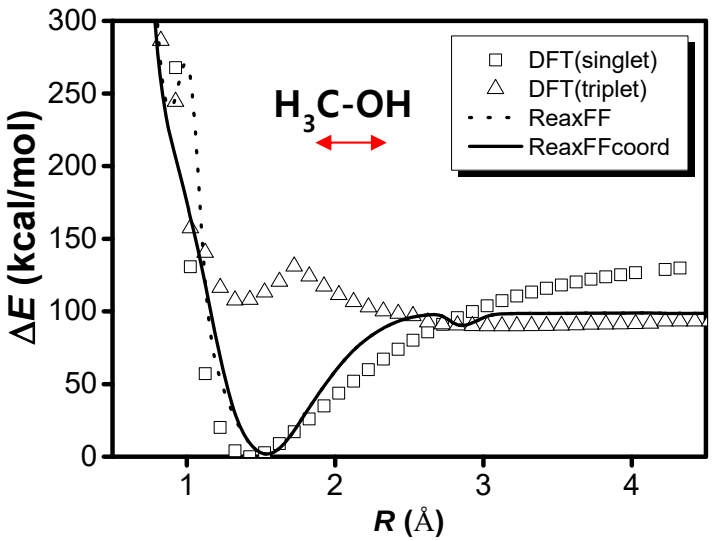

Figure S1. Dissociation energy curve of C-O bond in methanol (H_3COH).

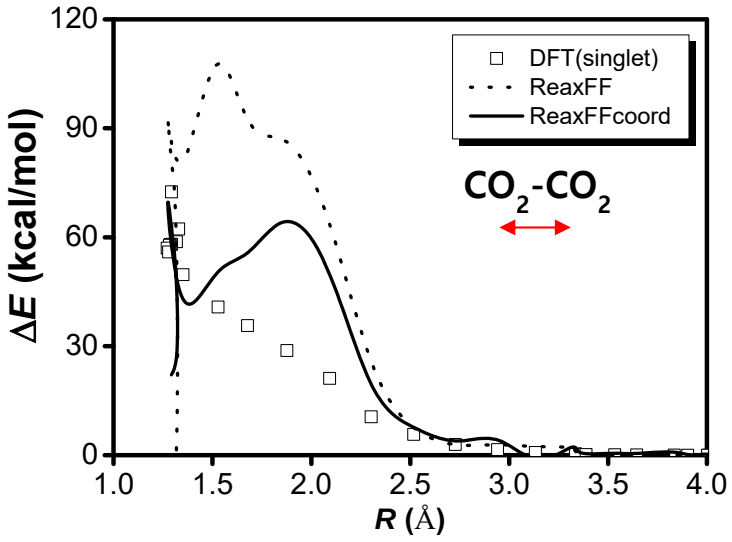

Figure S2. Dissociation energy curve for the intermolecular interaction between two CO_2 molecules.

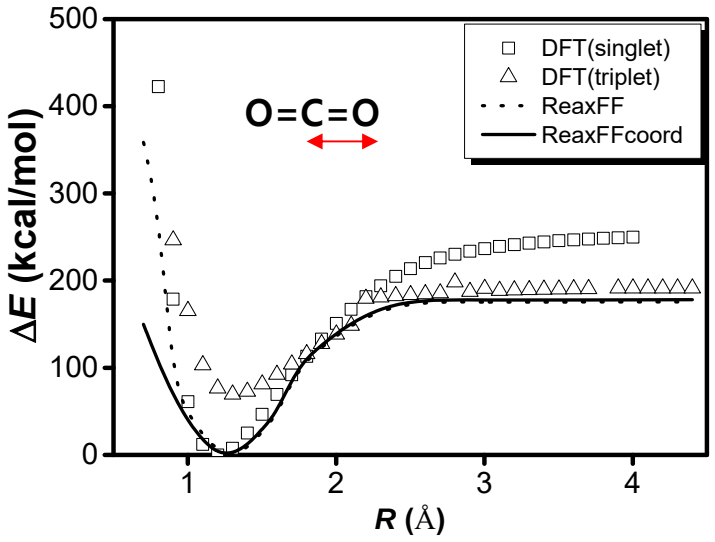

Figure S3. Dissociation energy curve of a C=O bond in CO_2.

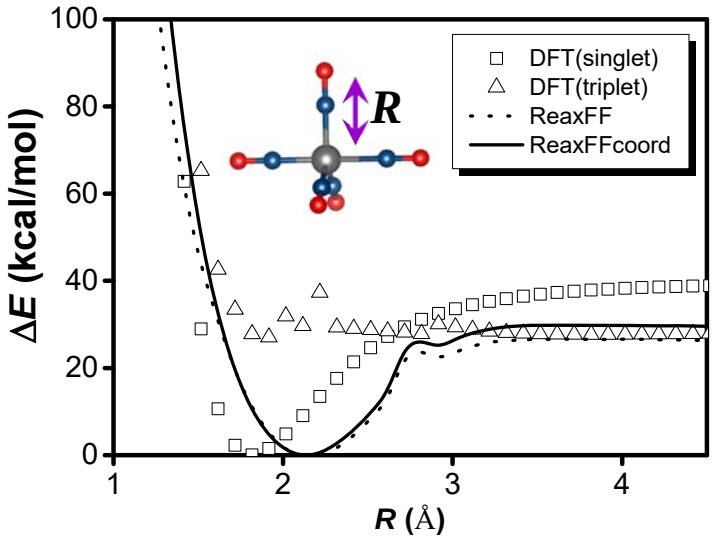

Figure S4. Dissociation energy curve of Fe-CO bond along the equatorial axis in $Fe(CO)_5$. This is different from Figure 1c that is for the dissociation along the axial axis.

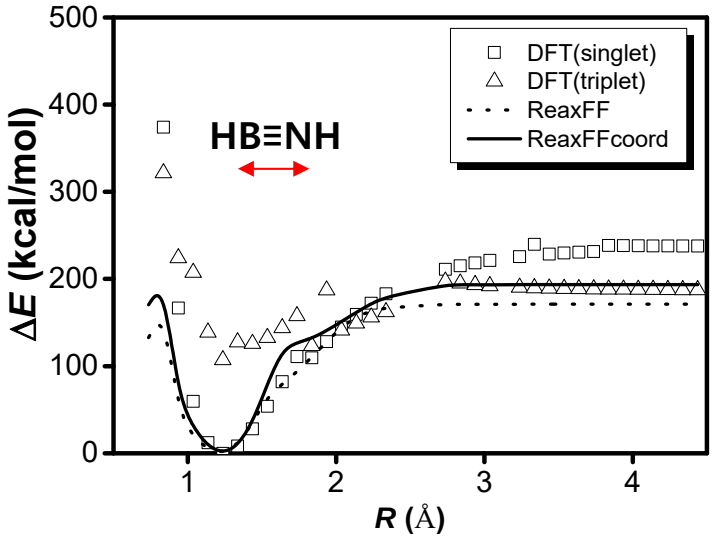

Figure S5. Dissociation energy curve for a B-N bond in HBNH molecule.

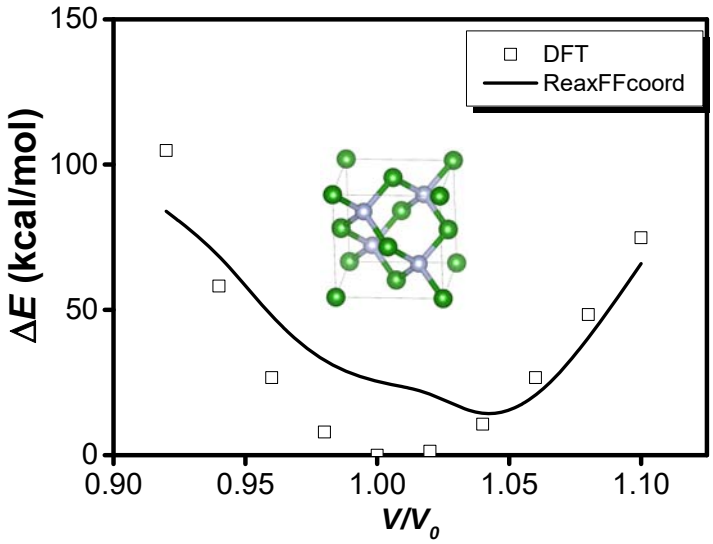

Figure S6. Equation of state (EOS) for *c*-BN.

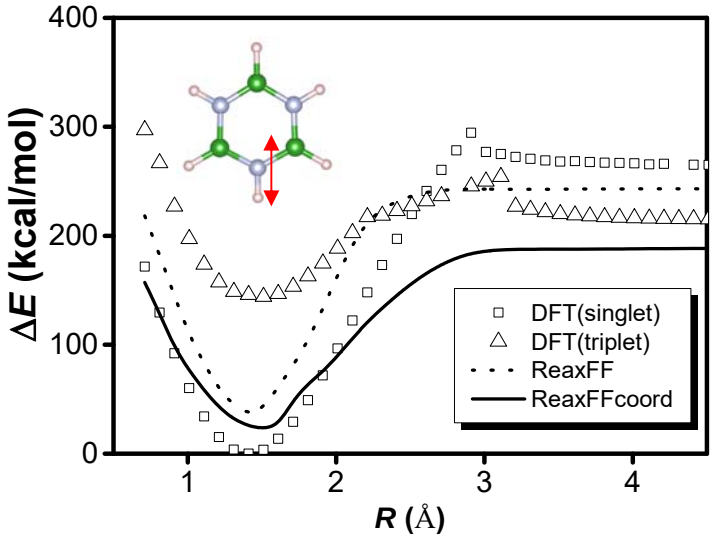

Figure S7. Dissociation energy curve of B-N bond in borazine ($B_3N_3H_6$).

Table S1. ReaxFF$_{coord}$ parameters for Fe/C/O system

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Reactive MD-force field: Fe/C/O
 39                ! Number of general parameters
    50.0000 !Overcoordination
     9.5469 !Overcoordination
     1.6725 !Valency
     1.7224 !Triple
     6.8702 !Triple
    60.4850 !C2-correction
     1.0588 !Undercoordination
     4.6000 !Triple
    12.1176 !Undercoordination
    13.3056 !Undercoordination
   -55.1978 !Triple
     0.0000 !Lower
    10.0000 !Upper
     2.8793 !Not
    33.8667 !Valency
     6.0891 !Valency
     1.0563 !Valency
     2.0384 !Valency
     6.1431 !Not
     6.9290 !Double
     0.3989 !Double
     3.9954 !Double
    -2.4837 !Not
     5.7796 !Torsion
    10.0000 !Torsion
     1.9487 !Torsion
    -1.2327 !Conjugation
     2.1645 !Conjugation
     1.5591 !vdWaals
     0.1000 !Cutoff
     1.7602 !Valency
     0.6991 !Overcoordination
    50.0000 !Overcoordination
     1.8512 !Valency
     0.5000 !Not
    20.0000 !Not
     5.0000 !Molecular
     0.0000 !Molecular
     0.7903 !Valency
  8            ! 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      0.8930     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    61.6606     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    59.0626     3.5027     0.7640     0.0021     0.9745     0.0000
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     -3.5500    2.9000    1.0493    4.0000    2.9225    0.0000    0.0000    0.0000
Fe    1.9306    3.0000   55.8450    2.1229    0.1163    0.4744   -1.6836    3.0000
     10.4193    7.0680    3.0000    0.0000   18.3725    1.7785    8.6281    0.0000
     -1.2000    0.0000   66.4838   25.3430   10.1260    0.7590    0.8563    0.0000
    -16.0573    2.6997    1.0338    6.0000    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
Si    2.1932    4.0000   28.0600    1.8951    0.1737    0.8112    1.2962    4.0000
     11.3429    5.2054    4.0000   21.7115  139.9309    4.0081    5.7104    0.0000
     -1.0000    0.0000  128.2031    9.0751   23.8188    0.8381    0.8563    0.0000
     -4.1684    2.0754    1.0338    4.0000    2.5791    1.4000    0.2000   13.0000
Al    2.1967    3.0000   26.9820    2.3738    0.2328    0.4265   -1.6836    3.0000
      9.4002    3.9009    3.0000    0.0076   16.5151    1.7429    6.8319    0.0000
     -1.0000    0.0000   78.4675   20.0000    0.2500    0.0000    0.8563    0.0000
    -22.7101    1.7045    1.0338    8.0000    2.5791    1.4000    0.2000   13.0000
X    -0.1000    2.0000    1.0080    2.0000    0.0000    0.4744   -0.1000    6.0000
     10.0000    2.5000    4.0000    0.0000    0.0000    4.0000   15.0000    0.0000
     -0.1000    0.0000  127.6226    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
25                ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                                pbe2;pbo3;pbo4;Etrip;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   2 153.3934    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
 1   3 164.4303   82.6772   75.1544   -0.3739   -0.1849    1.0000   10.4529    1.0000
           0.4475   -0.2288    7.0250    1.0000   -0.1363    4.8734    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   4 113.1509    0.0000    0.0000    0.6400   -0.3000    1.0000   36.0000    0.0100
           1.0000   -0.3500   15.0000    1.0000   -0.1450    4.1504    1.0000    0.0000
 2   4  78.2669    0.0000    0.0000    0.4668    0.0000    1.0000    6.0000    0.1766
           0.5673    1.0000    0.0000    1.0000   -0.1543    5.4965    0.0000    0.0000
 3   4  77.2864    0.0000    0.0000    0.3288   -0.3000    1.0000   36.0000    0.1023
           1.0000   -0.3500   15.0000    1.0000   -0.1109    7.6514    1.0000    0.0000
 4   4  44.2147    0.0000    0.0000    0.2236   -0.2000    0.0000   16.0000    0.2849
           0.4922   -0.2000   15.0000    1.0000   -0.0552    6.7583    0.0000    0.0000
 2   5 109.1686    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   5   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   5   0.0000    0.0000    0.0000    0.2500   -0.2000    0.0000   16.0000    0.5000
           0.5000   -0.2000   15.0000    1.0000   -0.2000   10.0000    0.0000    0.0000
 5   5   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   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   6 250.0000    0.0000    0.0000   -0.7128    0.0000    1.0000    6.0000    0.1186
          18.5790    1.0000    0.0000    1.0000   -0.0731    7.4983    0.0000    0.0000
 3   6 261.9074    5.9533    0.0000   -0.6223   -0.3000    1.0000   36.0000    0.7275
          10.1541   -0.2366   29.7817    1.0000   -0.1083    8.5924    6.0658    0.0000
 4   6   0.0000    0.0000    0.0000    1.0000    0.3000    0.0000   26.0000    1.0000
           0.5000    0.0000   12.0000    1.0000   -0.2000   10.0000    0.0000    0.0000
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 6  6   70.9120   54.0531   30.0000    0.4931   -0.3000    1.0000   16.0000    0.0392
          0.2476   -0.8055    7.1248    1.0000   -0.1009    8.7229    0.0000    0.0000
 1  7    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  7    0.8579    0.0000    0.0000   -0.6528   -0.3000    0.0000   36.0000    0.1551
         10.0663   -0.3500   25.0000    1.0000   -0.0842    7.1758    0.0000    0.0000
 3  7  227.9327    0.0000    0.0000   -0.8375   -0.3000    0.0000   36.0000    0.1286
          0.3686   -0.3500   25.0000    1.0000   -0.1740    5.2057    0.0000    0.0000
 4  7    0.0000    0.0000    0.0000    1.0000    0.3000    0.0000   26.0000    1.0000
          0.5000    0.0000   12.0000    1.0000   -0.2000   10.0000    0.0000    0.0000
 6  7    0.0000    0.0000    0.0000    1.0000    0.3000    0.0000   26.0000    1.0000
          0.5000    0.0000   12.0000    1.0000   -0.2000   10.0000    0.0000    0.0000
 7  7   34.0777    0.0000    0.0000    0.4832   -0.3000    0.0000   16.0000    0.5154
          6.4631   -0.4197   14.3085    1.0000   -0.1463    6.1608    0.0000    0.0000
17          ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2    0.1239    1.4004    9.8467    1.1210   -1.0000   -1.0000
 2  3    0.0283    1.2885   10.9190    0.9215   -1.0000   -1.0000
 1  3    0.1345    1.8422    9.7725    1.2835    1.1576   -1.0200
 1  4    0.3999    1.4558   11.0036    1.3918   -1.0000   -1.0000
 2  4    0.0200    1.9451   10.8595    1.4157   -1.0000   -1.0000
 3  4    0.0502    1.3407   10.1767    1.7735   -1.0000   -1.0000
 2  5    0.0568    1.6740    9.6297    1.2200   -1.0000   -1.0000
 3  5    0.1927    2.2551   11.2308   -1.0000   -1.0000   -1.0000
 4  5    0.1500    2.1500   11.0000   -1.0000   -1.0000   -1.0000
 1  6    0.2000    1.9000   12.0000   -1.0000   -1.0000   -1.0000
 2  6    0.1043    1.5000   11.8720    1.3005   -1.0000   -1.0000
 3  6    0.2000    1.9048   10.8374    1.7163    1.2444   -1.0000
 4  6    0.1000    2.0000   11.0000   -1.0000   -1.0000   -1.0000
 1  7    0.2000    1.9000   12.0000   -1.0000   -1.0000   -1.0000
 2  7    0.0564    1.4937   12.0744    1.7276   -1.0000   -1.0000
 3  7    0.1745    1.8928   11.2476    1.5382   -1.0000   -1.0000
 6  7    0.0295    1.5025   11.8687   -1.0000   -1.0000   -1.0000
66          ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
 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   53.9517    7.8968    2.6122    0.0000    3.0000   58.6562    1.0338
 3  1  3   76.9627   44.2852    2.4177  -25.3063    1.6334  -50.0000    2.7392
 2  1  3   65.0000   16.3141    5.2730    0.0000    0.4448    0.0000    1.4077
 1  3  1   72.6199   42.5510    0.7205    0.0000    2.9294    0.0000    1.3096
 1  3  3   81.9029   32.2258    1.7397    0.0000    0.9888   68.1072    1.7777
 3  3  3   80.7324   30.4554    0.9953    0.0000    3.0000   50.0000    1.0783
 1  3  2   70.1101   13.1217    4.4734    0.0000    0.8433    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   25.0000    3.0000    0.0000    1.0000    0.0000    1.0400
 3  2  3    0.0000   15.0000    2.8900    0.0000    0.0000    0.0000    2.8774
 2  2  3    0.0000    8.5744    3.0000    0.0000    0.0000    0.0000    1.0421
 1  4  1    7.0546   39.3227    1.0694    0.0000    0.7210    0.0000    3.1133
 1  1  4   29.2291   39.0677    1.2584    0.0000    0.0100    0.0000    1.6263
 1  4  4   47.3783    1.0170    7.8341    0.0000    2.8546    0.0000    1.0000
 4  1  4   33.2812   34.6443    3.0111    0.0000    0.1701    0.0000    1.0510
 2  1  4    0.0100   25.4983    1.5660    0.0000    0.0839    0.0000    1.2521
 2  4  2   20.3683    0.0100    2.2825    0.0000    0.7660    0.0000    1.3788
 2  2  4    0.0000    0.0100    1.0568    0.0000    1.8595    0.0000    3.6142
 4  2  4    0.0000   10.4428    7.9607    0.0000    2.3717    0.0000    1.1970
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 2   4   4   48.4128     4.0632     0.6773     0.0000     2.2274     0.0000     1.8605
 2   4   4  180.0000    -5.3883    21.7804     0.0000     0.5866     0.0000     1.0000
 1   3   4   90.0000    38.8254     7.9000     0.0000     2.9529     0.0000     1.4940
 3   1   4   30.5955    36.1214     8.0000     0.0000     0.1032     0.0000     1.0000
 3   4   3   47.8282     0.0100     1.9197     0.0000     0.1248     0.0000     2.5839
 4   3   4   43.8679    14.3345     8.0000     0.0000     0.0636     0.0000     1.6997
 2   3   4   26.0012    49.6772     0.0500     0.0000     1.1589     0.0000     1.0000
 3   3   4   73.6721    32.6330     1.7223     0.0000     1.0221     0.0000     1.4351
 3   4   4   68.7142     3.0974     8.0000     0.0000     0.0907     0.0000     1.0000
 3   2   4    0.0000     0.0100     3.2567     0.0000     2.0582     0.0000     1.3513
 2   4   3   38.5594    11.2599     0.1898     0.0000     0.1904     0.0000     1.4041
 3   2   5    0.0000     0.0100     0.5211     0.0000     0.0000     0.0000     1.3859
 1   4   2   44.2808     0.3810     0.0100     0.0000     0.2603     0.0000     1.9721
 1   2   4    0.8171     0.0100     2.8321     0.0000     2.4786     0.0000     2.3245
 6   6   6   78.5339    36.4328     1.0067     0.0000     0.1694     0.0000     1.6608
 2   6   6   77.2616     5.0190     7.8944     0.0000     4.0000     0.0000     1.0400
 2   6   2   75.7983    14.4132     2.8640     0.0000     4.0000     0.0000     1.0400
 3   6   6   90.6812    31.1846     4.4543     0.0000     0.5073     0.0000     2.1809
 2   6   3   73.6998    40.0000     1.8782     0.0000     4.0000     0.0000     1.1290
 3   6   3   80.1361    36.2368     0.9504     0.0000     0.2624     0.0000     2.0787
 6   3   6   80.4450     6.0739     1.7731     0.0000     3.2548     0.0000     1.0422
 2   3   6   86.7611     7.1742     1.4013     0.0000     1.4999     0.0000     1.0400
 3   3   6  103.4529    26.9589     1.3470     0.0000     1.7728     0.0000     1.3091
 2   2   6    0.0000    47.1300     6.0000     0.0000     1.6371     0.0000     1.0400
 6   2   6    0.0000    27.4206     6.0000     0.0000     1.6371     0.0000     1.0400
 3   2   6    0.0000     5.0000     1.0000     0.0000     1.0000     0.0000     1.2500
 3   2   7    0.0000     4.2750     1.0250     0.0000     1.3750     0.0000     1.4750
 2   2   7    0.0000     3.0000     1.0000     0.0000     1.0000     0.0000     1.2500
 7   2   7    0.0000    20.2391     0.1328     0.0000     2.9860     0.0000     1.0870
 2   3   7   90.0000    19.7491     1.8227     0.0000     1.0000     0.0000     2.5337
 3   3   7   34.4326    25.9544     5.1239     0.0000     2.7500     0.0000     1.7141
 7   3   7   23.7270    19.5973     4.0000     0.0000     0.6619     0.0000     1.9380
 2   7   2   67.4229     4.5148     5.9702     0.0000     3.0000     0.0000     2.6879
 2   7   3   41.8108    17.3800     2.6618     0.0000     0.7372     0.0000     1.0100
 3   7   3   54.0864     9.7594     1.9476     0.0000     3.0000     0.0000     1.4400
 2   7   7  180.0000   -26.7860     7.3549     0.0000     1.0000     0.0000     1.0252
 2   7   7   78.2279    37.6504     0.4809     0.0000     1.0000     0.0000     2.9475
 6   3   7   15.7093     0.0100     2.7033     0.0000     1.0000     0.0000     1.0000
 3   6   7   88.2703     0.3954     0.2500     0.0000     0.5000     0.0000     2.1060
 3   7   6   83.8306     0.3712     0.2500     0.0000     0.5000     0.0000     2.1153
33          ! 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    1.2799    20.7787    -0.5249    -2.5000    -1.0000     0.0000     0.0000
 2   1   1   3    1.9159    19.8113     0.7914    -4.6995    -1.0000     0.0000     0.0000
 3   1   1   3   -1.4477    16.6853     0.6461    -4.9622    -1.0000     0.0000     0.0000
 1   1   3   1    0.4816    19.6316    -0.0057    -2.5000    -1.0000     0.0000     0.0000
 1   1   3   2    1.2044    80.0000    -0.3139    -6.1481    -1.0000     0.0000     0.0000
 2   1   3   1   -2.5000    31.0191     0.6165    -2.7733    -2.9807     0.0000     0.0000
 2   1   3   2   -2.4875    70.8145     0.7582    -4.2274    -3.0000     0.0000     0.0000
 1   1   3   3   -0.3566    10.0000     0.0816    -2.6110    -1.9631     0.0000     0.0000
 2   1   3   3   -1.4383    80.0000     1.0000    -3.6877    -2.8000     0.0000     0.0000
 3   1   3   1   -1.1390    78.0747    -0.0964    -4.5172    -3.0000     0.0000     0.0000
 3   1   3   2   -2.5000    70.3345    -1.0000    -5.5315    -3.0000     0.0000     0.0000
 3   1   3   3   -2.0234    80.0000     0.1684    -3.1568    -2.6174     0.0000     0.0000
 1   3   3   1    1.1637   -17.3637     0.5459    -3.6005    -2.6938     0.0000     0.0000
 1   3   3   2   -2.1289    12.8382     1.0000    -5.6657    -2.9759     0.0000     0.0000
 2   3   3   2    2.5000   -22.9397     0.6991    -3.3961    -1.0000     0.0000     0.0000
```

```
1   3   3   3     2.5000 -25.0000     1.0000   -2.5000   -1.0000     0.0000     0.0000
2   3   3   3    -2.5000   -2.5103   -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    0.0000     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
2   6   6   2     0.0000    0.0000    0.0640   -2.4426    0.0000     0.0000     0.0000
2   6   6   6     0.0000    0.0000    0.1587   -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
2   1   4   4     0.0000    0.0000    0.0000   -5.0000    0.0000     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
1     ! Nr of coordinate covalent bonds; r0cob;pcb1;pcb2,Decb,valcb
1   3     1.0545   -0.2391   10.1856   12.3861    1.0000
```

Table S2. ReaxFF$_{cood}$ force field parameters for C/H/B/N system

```
Reactive MD-force field: C/H/B/N
 39                    ! Number of general parameters
    50.0000 !Overcoordination
     9.5469 !Overcoordination
    26.5405 !Valency
     1.7224 !Triple
     6.8702 !Triple
    60.4850 !C2-correction
     1.0588 !Undercoordination
     4.6000 !Triple
    12.1176 !Undercoordination
    13.3056 !Undercoordination
   -70.5044 !Triple
     0.0000 !Lower
     8.0000 !Upper
     2.8793 !Not
    33.8667 !Valency
     6.0891 !Valency
     1.0563 !Valency
     2.0384 !Valency
     6.1431 !Not
     6.9290 !Double
     0.3989 !Double
     3.9954 !Double
    -2.4837 !Not
     5.7796 !Torsion
    10.0000 !Torsion
     1.9487 !Torsion
    -1.2327 !Conjugation
     2.1645 !Conjugation
     1.5591 !vdWaals
     0.0010 !Cutoff
     2.1365 !Valency
     0.6991 !Overcoordination
    50.0000 !Overcoordination
     1.8512 !Valency
     0.5000 !Not
    20.0000 !Not
     5.0000 !Molecular
     0.0000 !Molecular
     2.6962 !Valency
  4                 ! Nr of atoms; ro,s;val;a.m;Rvdw;Evdw;gammaEEM;ro,p;val(e)
                    alfa;gammavdW;val(angle);pvoun5;n.u.;chiEEM;etaEEM;n.u.
                    ro,pp;plp2;HeatInc;pboc4;pboc3;pboc5;n.u.;n.u.
                    povun2;pval3(ang);n.u.;val(boc);pval5(ang);n.u.;n.u.;n.u.
 C      1.3825     4.0000    12.0000     1.9133     0.1853     0.9000     1.1359     4.0000
        9.7602     2.1346     4.0000    33.2433    79.5548     8.0066     6.8000     0.0000
        1.2104     0.0000   199.0303     8.6991    34.7289    13.3894     0.8563     0.0000
       -2.8983     2.5000     1.0564     4.0000     2.9663     1.4000     0.1000    10.0000
 H      0.6867     1.0000     1.0080     1.3525     0.0616     0.7492    -0.1000     1.0000
        9.3858     5.0013     1.0000     0.0000   121.1250     6.5362     7.0327     1.0000
       -0.1000     0.0000    59.5599     6.1752     4.8714     0.0009     1.0698     0.0000
      -15.7683     2.1504     1.0338     1.0000     2.8793     0.6000     0.1000    10.0000
 B      1.2610     3.0000    10.8110     1.7215     0.0550     0.9088     0.9359     3.0000
       12.4662     2.9393     3.0000     7.2404    80.0000     6.8775     6.7020     0.0000
       -1.3000     0.0000    -2.3700     3.6849     7.4347     1.0943     0.0000     0.0000
```

```
     -3.6082     1.6200     1.0564     3.0000     2.8413     1.4000     0.1000    12.0000
N     1.5299     3.0000    14.0000     1.8354     0.0135     1.0000     1.3905     5.0000
      9.7119     8.4575     4.0000    27.4217   100.0000     8.1308     7.0000     2.0000
      1.2069    26.9280    -2.3700     2.3279     3.0410     2.6432     0.9745     0.0000
     -6.4340     2.3842     1.0183     4.0000     2.8793     1.4000     0.1000    10.0000
10                    ! Nr of bonds; Edis1;Edis2;Edis3;pbe1;pbo5;13corr;pbo6;povu
                                      pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr;n.u.
 1   1 156.5953 100.0397    80.0000    -0.8157    -0.4591     1.0000    37.7369     0.4235
           0.4527    -0.1000     9.2605     1.0000    -0.0750     6.8316     1.0000     0.0000
 1   2 164.4970     0.0000     0.0000    -0.4426     0.0000     1.0000     6.0000     0.6668
           6.2320     1.0000     0.0000     1.0000    -0.0476     5.5015     0.0000     0.0000
 2   2 165.7021     0.0000     0.0000    -0.8238     0.0000     1.0000     6.0000     0.3597
           6.5603     1.0000     0.0000     1.0000    -0.0113     5.6991     0.0000     0.0000
 1   3 182.8256 134.3150     0.0000    -0.7467    -0.3388     1.0000    30.7152     0.2751
           0.5734    -0.2121    11.6795     1.0000    -0.1374     5.9223     1.0000     0.0000
 2   3 177.4103     0.0000     0.0000    -0.4601    -0.3000     1.0000    25.0000     0.4971
           9.2806     0.0000     0.0000     1.0000    -0.0722     5.1245     1.0000     0.0000
 3   3   98.1913     0.0000     0.0000     0.9895    -0.2500     1.0000    25.0000     0.0988
           0.7482    -0.2000    15.0000     1.0000    -0.1527     5.4170     1.0000     0.0000
 1   4 187.3038 101.8119 118.7455    -0.9626    -0.2187     1.0000     8.3529     0.4161
           0.4543    -0.4591    21.7699     1.0000    -0.1244     6.2791     1.0000     0.0000
 2   4 231.8918     0.0000     0.0000    -0.7398     0.0000     1.0000     6.0000     0.4224
           9.1469     1.0000     0.0000     1.0000    -0.0491     5.7202     0.0000     0.0000
 3   4 101.0691 146.9351     0.0000     0.9000    -0.2500     1.0000    25.0000     0.1083
           0.3777    -0.4268    11.7687     1.0450    -0.1826     5.9713     1.0000     0.0000
 4   4 115.0457    94.4037 166.9967    -0.9395    -0.2538     1.0000    13.2393     1.0000
           0.2951    -0.4426     8.9359     1.0198    -0.1805     5.0773     1.0000     0.0000
 6                 ! Nr of off-diagonal terms;a1;a2;Dij;RvdW;alp;ros;rop;ropp
 1   2     0.0415     1.6927    10.3459     1.0426    -1.0000    -1.0000
 1   3     0.1329     1.8035    11.0558     1.3418     0.9000    -1.0000
 2   3     0.0526     1.5010    11.2019     1.1648    -1.0000    -1.0000
 1   4     0.1115     1.7854    10.2359     1.3643     1.2674     0.9778
 2   4     0.0367     1.6470    10.5106     0.9496    -1.0000    -1.0000
 3   4     0.1592     1.6069     9.8569     1.4845     1.3464    -1.0000
36                 ! Nr of angles;a1;a2;a3;Tho;pva1;pva2;pcoa1;pva7;ppen1;pva4
 1   1   1   67.2326    22.0695     1.6286     0.0000     1.7959    15.4141     1.8089
 1   1   2   69.6421     9.2578     3.6521     0.0000     0.0058     0.0000     1.0400
 2   1   2   75.4958    14.5436     2.7438     0.0000     0.0127     0.0000     1.0400
 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
 2   3   2   62.5987    14.6089     2.3811     0.0000     3.0000     0.0000     3.0000
 2   3   3   55.0000    32.2012     4.7029     0.0000     3.0000     0.0000     1.0400
 2   2   3    0.0000     5.0019     1.0000     0.0000     0.0000     0.0000     1.5000
 3   2   3    0.0000     5.0000     1.0000     0.0000     1.0000     0.0000     1.0400
 1   1   3   55.2354     4.8896     1.1332     0.0000     1.5533     0.0000     0.9657
 1   3   1   30.4469     2.9502     1.9735     0.0000     2.3791     0.0000     1.1179
 3   1   3   51.2292    14.2777     0.8300     0.0000     1.7820     0.0000     0.8913
 2   1   3   68.7093     3.5601     3.5152     0.0000    -0.1213     0.0000     1.3713
 1   3   2   71.1954    22.6026     3.1828     0.0000     0.0130     0.0000     1.1667
 1   3   3   27.0691    11.9197     0.9805     0.0000     1.0377     0.0000     1.1300
 3   3   3   70.0000    35.0000     3.0000     0.0000     1.5000     0.0000     1.0100
 2   1   4   43.8591     5.2941     0.5853     0.0000     0.7547     0.0000     0.6289
 1   4   2   92.3431    14.6346     1.5505     0.0000     0.9201     0.0000     0.6889
 2   4   4   72.7618    24.2550     2.3034     0.0000     0.1000     0.0000     1.0400
 2   4   2   85.5836    27.9831     4.0538     0.0000     0.7544     0.0000     1.2487
 4   2   4    0.0000     5.0000     2.0000     0.0000     0.0000     0.0000     1.0400
 2   2   4    0.0000    10.0019     1.0000     0.0000     0.0000     0.0000     1.0400
 2   4   3   55.0000     2.5000     0.1000     0.0000     0.1000     0.0000     2.2627
```

```
 2  3  4   55.0000    2.5000    0.1000    0.0000    0.1000    0.0000    2.2627
 4  3  4   70.6534   33.9304    3.8331    0.0000    0.9534    0.0000    1.4384
 3  4  3   60.4791   17.9894    0.9923    0.0000    3.5600    0.0000    1.2797
 3  2  4    0.0000    9.6980    1.0000    0.0000    1.0000    0.0000    1.0400
 4  4  4   70.0000   35.0000    3.0000    0.0000    1.5000    0.0000    1.0100
 1  4  1   62.2681    7.7197    0.0207    0.0000    1.5838    0.0000    1.0430
 4  1  4  110.1539   12.1105    2.4783    0.0000    1.5624    0.0000    0.9905
 1  1  4   50.2255   12.7546    0.9761    0.0000    1.5333    0.0000    1.0500
 1  4  4   60.1844   10.6877    0.3922    0.0000    1.1860    0.0000    1.0500
 1  3  4   45.0029   18.6356    0.9204    0.0000    1.1613    0.0000    1.1158
 1  4  3   44.0283   -0.3928   -0.3598    0.0000    1.0159    0.0000    0.9794
 3  1  4   54.1678   16.3254    0.5841    0.0000    1.0956    0.0000    1.0026
36                 ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;ptor1;pcot1;n.u.
 1  1  1  1  -0.2500   11.5822    0.1899   -4.7057   -2.2047    0.0000    3.6702
 1  1  1  2   0.0000   49.1001    0.2713   -8.5284   -1.5309    0.0000    0.0000
 2  1  1  2   0.0000   34.0265    0.3804   -6.3917   -0.9965    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  4  0   0.0000    0.1000    0.0200   -2.5415    0.0000    0.0000    0.0000
 0  4  4  0  -2.0000   24.4048   -0.1617   -3.3327   -2.0000    0.0000    0.0000
 4  3  4  3  -0.2500   11.5822    0.1899   -4.7057   -2.2047    0.0000    3.6702
 0  3  4  0  -2.0000   19.3351    0.3228   -5.4735    0.0000    0.0000    0.0000
 0  3  3  0   0.2500   50.0000    0.3000   -7.5000    0.0000    0.0000    0.0000
 2  3  4  2  -0.1007   23.8639    0.3443   -3.0822   -5.8276    0.0000    0.0000
 1  1  1  3  -0.1100   34.6047   -0.0128   -5.9379   -1.9886    0.0000    0.0000
 3  1  1  3  -0.2500   34.7453    0.0288   -6.3507   -1.6000    0.0000    0.0000
 1  1  3  1  -0.2500   34.7453    0.0288   -6.3507   -1.6000    0.0000    0.0000
 1  1  3  2   0.0000   49.1001    0.2713   -8.5284   -1.5309    0.0000    0.0000
 2  1  3  1   0.0000   49.1001    0.2713   -8.5284   -1.5309    0.0000    0.0000
 2  1  3  2  -0.1491   23.9139    0.3015   -3.2203   -5.7735    0.0000    0.0000
 1  1  3  3  -0.5888   34.6343   -0.3716   -6.4877   -1.5764    0.0000    0.0000
 2  1  1  3   0.0000   50.0000    0.3000   -4.0000   -2.0000    0.0000    0.0000
 2  1  3  3  -0.2500   34.7453    0.0288   -6.3507   -1.6000    0.0000    0.0000
 3  1  3  1  -0.3461   34.1343   -1.0446  -10.9658   -1.8018    0.0000    0.0000
 1  3  3  3  -0.7796   35.3481    0.5161   -5.2825   -1.5504    0.0000    0.0000
 2  1  4  2   0.0134   34.0609   -0.0630   -6.0516   -1.2887    0.0000    0.0000
 1  1  1  4  -0.0888   34.8553    0.0670   -6.3632   -1.5765    0.0000    0.0000
 1  1  4  4  -0.6800   34.7750   -0.0114   -6.4101   -1.0960    0.0000    0.0000
 1  4  4  4  -0.2928   34.9471   -0.0729   -6.4675   -1.4813    0.0000    0.0000
 4  1  4  1  -0.2001   36.9660    0.0938   -6.7107   -1.3023    0.0000    0.0000
 1  4  4  1  -0.2000   34.7042   -0.3758   -6.6607   -1.7959    0.0000    0.0000
 4  1  1  4  -0.2039   34.9911   -0.2512   -6.0767   -1.2376    0.0000    0.0000
 1  1  4  1  -0.2259   34.8211    0.3488   -6.3307   -1.7320    0.0000    0.0000
 1  1  3  4  -1.1345   36.8371   -0.5533   -6.6298   -1.6621    0.0000    0.0000
 1  1  4  3  -0.7527   33.5523   -0.5207   -7.1302   -2.4036    0.0000    0.0000
 4  1  3  1  -0.4700   34.5453   -0.0112   -6.5507   -1.7000    0.0000    0.0000
 3  1  4  1  -0.1150   34.8425    0.1065   -6.4788   -1.7339    0.0000    0.0000
 1  3  4  1  -0.9249   33.8546    0.6616   -7.2472   -0.9719    0.0000    0.0000
 3  1  1  4  -0.1305   34.7103   -0.4508   -6.8580   -1.7917    0.0000    0.0000
 1                 ! Nr of hydrogen bonds;at1;at2;at3;r(hb);p(hb1);p(hb2);p(hb3)
 4  2  4    2.0000   -2.5002    3.0000   15.0000
 1       ! Nr of coordinate covalent bonds; r0cob;pcb1;pcb2,Decb,valc
 3  4    1.3411   -0.0518    9.4954   15.3418    1.0000
```

S2. Additional description for ReaxFF$_{coord}$

The system energy of ReaxFF (E_{system}) is

$$E_{system} = E_{bond} + E_{over} + E_{under} + E_{lp} + E_{triple} + E_{val} + E_{pen} + E_{tors} + E_{conj} + E_{hb} + E_{vdW} + E_{Coulomb}$$

(S1)

On the other hand, the system energy for ReaxFF$_{coord}$ is

$$E_{system} = E_{bond} + E_{over} + E_{under} + E_{lp} + \boldsymbol{E_{coord}} + E_{triple} + E_{val} + E_{pen} + E_{tors} + E_{conj} + E_{hb} + E_{vdW} + E_{Coulomb} \quad \text{(S2)}$$

Here, note the position of E_{triple} just after E_{coord}, indicating that the calculation of E_{triple} is performed after that of E_{coord}.

We discuss this calculation sequence with an example of ammonia borane (**AB**). In contrast to the original ReaxFF scheme,[S5-S7] the bond list for a coordinate bond and the primitive bond order ($BO_{ij}^{\prime\prime cb}$) (Eq. 3 in the main text) for elements relevant to a coordinate bond are generated from the force field parameters, while the bond list and bond order (BO) for each bond are generated from the Verlet neighbor list in preparation for the E_{bond} calculation.

When the distance between B and N is r = 1.672 Å, $BO_{BN}^{\prime\prime cb}$ = 0.651 from Eq. 3. The necessary information for E_{coord} is obtained from the previous steps. VO_i can be obtained from the calculation of E_{bond}, and NL_i are calculated from E_{lp}. $VO_{opt,B}$ = 1, but VO_B = 0.812 for the optimized geometry; thus, f_a^{cb} = 0.965 from Eq. 5 in the main text, as shown in Figure S8.

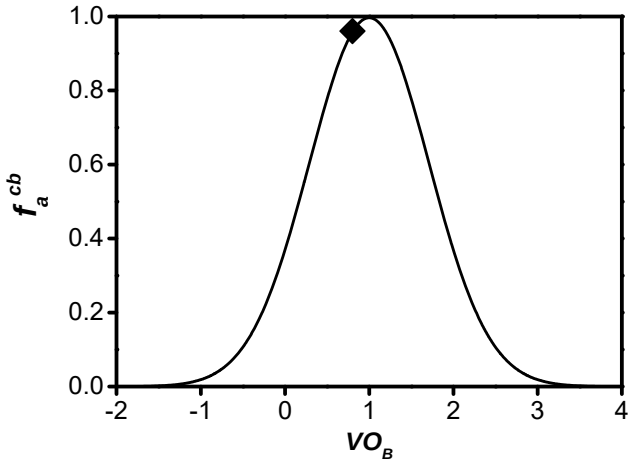

Figure S8. f_a^{cb} graph for $VO_{opt,i}$=1. A diamond is the position of f_a^{cb} for B in the optimized structure of **AB**.

Likewise, $NL_{opt,N}$ = 1, but VO_N = 0.729, thus f_d^{cb} = 0.929 from Eq. 6 in the main text, as shown in Figure S9.

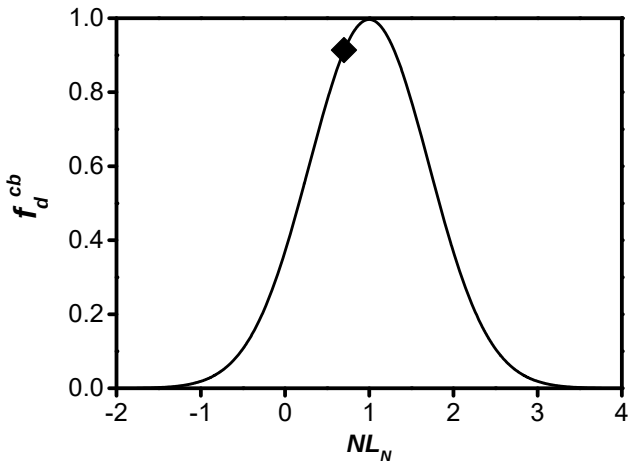

Figure S9. f_d^{cb} graph for $NL_{opt,i}$=1. A diamond is the position of f_d^{cb} for N in the optimized structure of **AB**.

NV_B and NV_N are equal to four as mentioned in the main text. For carbon (C) atom, it has four unpaired electrons and then can have four bonds, leading to $NV_C = 4$. For nitrogen (N) atom, it has 3 unpaired electrons and 1 lone pair, leading to the maximum valency of 4 (four bonds). Similarly, for oxygen (O) atom, it has 2 unpaired electrons and 2 lone pairs, leading to the maximum valency of 4. For boron (B) atom, it has 3 unpaired electrons, but it can have the maximum four chemical bonds, which is found in ammonia borane (NH_3BH_3) molecule or *c*-BN crystal. To explain this, we have introduced the vacant orbital concept and assumed that this vacant orbital also contributes to NV_i. Based on this fact, NV_B of B atom is defined as 4. Using the determined $BO_{ij}^{''cb}$, f_a^{cb} and f_d^{cb} values for B and N, $BO_{ij}^{'cb}$ can be calculated from Eq. 7 in the main text, leading to $BO_{ij}^{'cb} = 0.583$. The overcorrection function f_1 is similar to the equations of the original ReaxFF.[S5]

$$f_1(\Delta_i, \Delta_j) = \frac{1}{2}\left(\frac{val_i^{cb}+f_2(\Delta_i,\Delta_j)}{val_i^{cb}+f_2(\Delta_i,\Delta_j)+f_3(\Delta_i,\Delta_j)} + \frac{val_j^{cb}+f_2(\Delta_i,\Delta_j)}{val_j^{cb}+f_2(\Delta_i,\Delta_j)+f_3(\Delta_i,\Delta_j)}\right) \quad \text{(S3)}$$

$$f_2(\Delta_i, \Delta_j) = \exp(-p_{boc1}\Delta_i) + \exp(-p_{boc1}\Delta_j) \quad \text{(S4)}$$

$$f_3(\Delta_i, \Delta_j) = -\frac{1}{p_{boc2}}\ln\left\{\frac{1}{2}\left[\exp(-p_{boc2}\Delta_i) + \exp(-p_{boc2}\Delta_j)\right]\right\} \quad \text{(S5)}$$

$$\Delta_i = \sum_j^{neighbor} BO_{ij}^{'cb} - val_i^{cb} \quad \text{(S6)}$$

The bond order correction term in E_{bond} of ReaxFF consists of three auxiliary functions f_1, f_4 and f_5, where f_1 also includes f_2 and f_3.[S8] Thus, the correction term for E_{coord} also includes the f_2 and f_3 functions, which means that there exist three auxiliary functions for this term. While f_1 is for an overcoordination correction, f_4 and f_5 are used for softening the correction for atoms with lone pair electrons. In this work, only an overcoordination problem needs to be

solved in E_{coord} when atom i have many coordinate bonds, i.e., for crystal systems such as *c*-BN. f_4 and f_5 are excluded because treatment of lone pair electrons is explicitly included in E_{coord} functions.

Here, $val_B^{cb} = val_N^{cb} = 1$ from the force field parameter set in Table S2. Because $BO_{BN}^{\prime cb}$ = 0.583 is lower than $val_i^{cb} = 1$, there is no overcorrection; thus, f_1 = 1 and BO_{BN}^{cb} = 0.583 from Eq. 8 in the main text. Finally, E_{coord} = -8.95 from Eq. 9 in the main text.

S3. Reaction pathway between two AB molecules

From the *NVT* MD simulation using the developed $ReaxFF_{coord}$ for the **AB** bulk system in Figure 3d of the main text, we found that a $(BH_3)_2NH_3$ is generated. The structure is very similar to the **BBA-com + A** state of Nguyen et al.[S9] observed in the early stage of formation of the diammoniate of diborane ion pair isomer, $[BH_4]^-[NH_3BH_2NH_3]^+$ (**DADB**) from two **AB**s. Here, we reproduced their work by using the DFT method and compared the reaction pathway with that obtained by $ReaxFF_{coord}$ (Figure S10). Although the energy level determined by $ReaxFF_{coord}$ is slightly high due to the long-range distance between two **AB** molecules in the reactant state (**2AB**), the energy difference between the transition (**2AB-ts1**) and the product (**BBA-com+A)** states is very similar to that determined from the DFT calculation. This clearly supports the accuracy of the developed $ReaxFF_{coord}$.

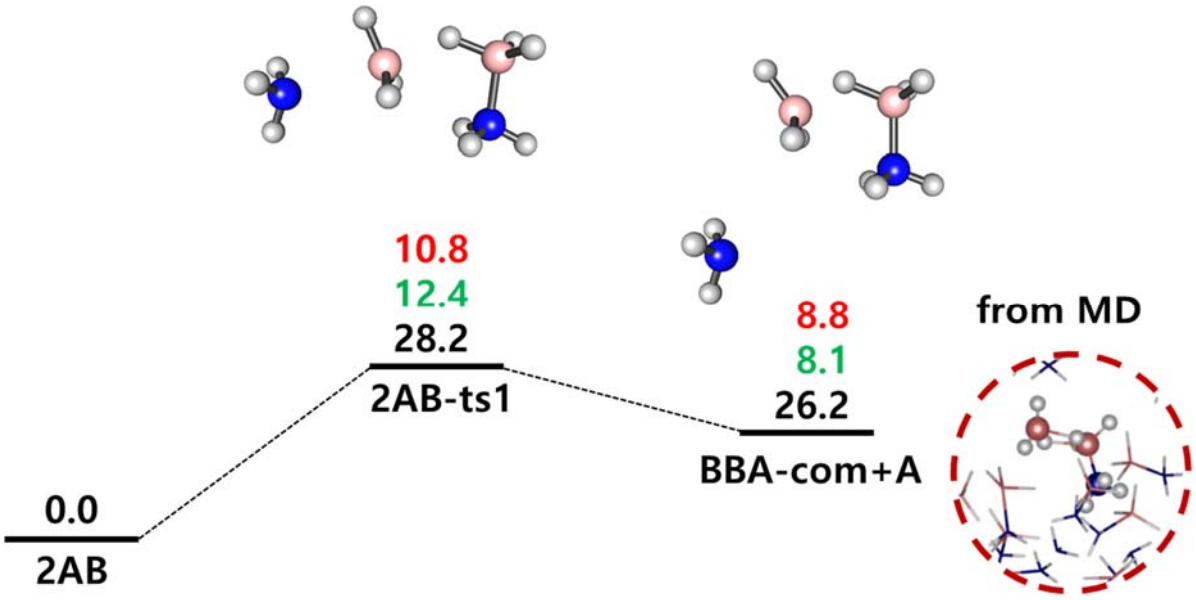

Figure S10. Reaction pathway for the formation of **DADB** occurring during B-N dissociation from 2**AB**. The name of each state is from Ref. S9. Energy values are in kcal/mol. The red energy value is for DFT, the black is for $ReaxFF_{coord}$, and the green is for ReaxFF reported in Ref. S9. For comparison, the results for $(BH_3)_2NH_3$ observed in our MD simulation with the $ReaxFF_{coord}$ is included in the inset.

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