# Support Information

## Highly Shocked Polymer Bonded Explosives at a Non-Planar Interface: Hotspot Formation leading to Detonation

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**Complete Parameters of ReaxFF Reactive Force Field for Si-PETN:**

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Reactive MD-force field: nitramines (RDX/HMX/TATB/PETN))+DMNA-barrier+innervdWaa
 39       ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.4514 !Overcoordination parameter
   29.8953 !Valency angle conjugation parameter
  216.5421 !Triple bond stabilisation parameter
   12.2245 !Triple bond stabilisation parameter
    0.0000 !C2-correction
    1.0701 !Undercoordination parameter
    7.5000 !Triple bond stabilisation parameter
   11.9083 !Undercoordination parameter
   13.3822 !Undercoordination parameter
  -10.9834 !Triple bond stabilization energy
    0.0000 !Lower Taper-radius
   10.0000 !Upper Taper-radius
    2.8793 !Not used
   33.8667 !Valency undercoordination
    3.3976 !Valency angle/lone pair parameter
    1.0563 !Valency angle
    2.0384 !Valency angle parameter
    6.1431 !Not used
    6.9290 !Double bond/angle parameter
    0.0283 !Double bond/angle parameter: overcoord
    0.0570 !Double bond/angle parameter: overcoord
   -2.4837 !Not used
    5.8374 !Torsion/BO parameter
   10.0000 !Torsion overcoordination
    1.8820 !Torsion overcoordination
   -1.2327 !Conjugation 0 (not used)
    2.1861 !Conjugation
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  1.5591 !vdWaals shielding
  0.0100 !Cutoff for bond order (*100)
  4.8414 !Valency angle conjugation parameter
  3.5857 !Overcoordination parameter
 38.6472 !Overcoordination parameter
  2.1533 !Valency/lone pair parameter
  0.5000 !Not used
  1.0000 !Scale factor (d) in dispersion
  5.0000 !Molecular energy (not used)
  0.0000 !Molecular energy (not used)
  6.9784 !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    1.3742   4.0000  12.0000   1.9684   0.1723   0.8712   1.2385   4.0000
     8.7696   0.1000   4.0000  31.0823  79.5548   5.7254   6.9235   0.0000
     1.2104   0.0000 183.8108   5.7419  33.3951  11.9957   0.8563   0.0000
    -2.8983   4.7820   1.0564   4.0000   2.9663   1.6737   0.1421  14.0707
     0.0001   1.9255
H    0.6867   1.0000   1.0080   1.3525   0.0616   0.8910  -0.1000   1.0000
     9.1506   0.1000   1.0000   0.0000 121.1250   3.8446  10.0839   1.0000
    -0.1000   0.0000  58.4369   3.8461   3.2540   1.0000   1.0698   0.0000
   -15.7683   2.1504   1.0338   1.0000   2.8793   1.2669   0.0139  12.4538
     0.0001   1.4430
O    1.3142   2.0000  15.9990   1.9741   0.0880   0.8712   1.1139   6.0000
     9.9926   0.1000   4.0000  29.5271 116.0768   8.5000   7.1412   2.0000
     0.9909  14.7235  69.2921   9.1371   1.6258   0.1863   0.9745   0.0000
    -3.5965   2.5000   1.0493   4.0000   2.9225   1.7221   0.1670  13.9991
   623.8417   1.7500
N    1.2456   3.0000  14.0000   2.0437   0.1035   0.8712   1.1911   5.0000
     9.8823   0.1000   4.0000  32.4758 100.0000   6.8453   6.8349   2.0000
     1.0636   0.0276 127.9672   2.2169   2.8632   2.4419   0.9745   0.0000
    -4.0959   2.0047   1.0183   4.0000   2.8793   1.5967   0.1649  13.9888
  1240.001    1.8300
S    1.9647   2.0000  32.0600   2.0783   0.2176   1.0336   1.5386   6.0000
     9.9676   0.0812   4.0000  35.1648 112.1416   6.5000   8.2545   2.0000
     1.4703   9.4922  70.0338   8.5146  28.0801   8.5010   0.9745   0.0000
   -10.0773   2.7466   1.0338   6.2998   2.8793   1.5967   0.1649  13.9888
   180.0000   2.0783
Si   2.0276   4.0000  28.0600   2.2042   0.1322   0.8218   1.5758   4.0000
    11.9413   0.0618   4.0000  11.8211 136.4845   1.8038   7.3852   0.0000
    -1.0000   0.0000 126.5331   6.4918   8.5961   0.2368   0.8563   0.0000
    -3.8112   3.1873   1.0338   4.0000   2.5791   1.0000   0.1649  13.9888
     0.0001   2.2042
X   -0.1000   2.0000   1.0080   2.0000   0.0000   1.0000  -0.1000   6.0000
```

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  10.0000   0.5000   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   1.5967   0.1649  13.9888
 180.0000   2.0000
20      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                  pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
 1  1 141.9346 113.4487  67.6027   0.1554  -0.3045   1.0000  30.4515   0.4283
      0.0801  -0.2113   8.5395   1.0000  -0.0933   6.6967   1.0000   0.0000
 1  2 155.7526   0.0000   0.0000  -0.4525   0.0000   1.0000   6.0000   0.5921
     12.1053   1.0000   0.0000   1.0000  -0.0097   8.6351   0.0000   0.0000
 2  2 169.8421   0.0000   0.0000  -0.3591   0.0000   1.0000   6.0000   0.7503
      9.3119   1.0000   0.0000   1.0000  -0.0169   5.9406   0.0000   0.0000
 1  3 157.7219  89.8921  27.9315  -0.4324  -0.1742   1.0000  15.0019   0.5160
      1.2934  -0.3079   7.0252   1.0000  -0.1543   4.5116   0.0000   0.0000
 3  3 108.9631 158.3501  42.0558   0.1226  -0.1324   1.0000  28.5716   0.2545
      1.0000  -0.2656   8.6489   1.0000  -0.1000   6.8482   1.0000   0.0000
 1  4 128.9104 171.2945 100.5836  -0.1306  -0.4948   1.0000  26.7458   0.4489
      0.3746  -0.3549   7.0000   1.0000  -0.1248   4.9232   1.0000   0.0000
 3  4  76.1062 118.8680  75.7263   0.7080  -0.1062   1.0000  16.6913   0.2407
      0.3535  -0.1906   8.4054   1.0000  -0.1154   5.6575   1.0000   0.0000
 4  4 160.6599  73.3721 154.2849  -0.7107  -0.1462   1.0000  12.0000   0.6826
      0.9330  -0.1434  10.6712   1.0000  -0.0890   4.6486   1.0000   0.0000
 2  3 230.7607   0.0000   0.0000  -0.6643   0.0000   1.0000   6.0000   0.9854
      5.1146   1.0000   0.0000   1.0000  -0.0532   5.1189   0.0000   0.0000
 2  4 208.0443   0.0000   0.0000  -0.3923   0.0000   1.0000   6.0000   0.3221
     10.5505   1.0000   0.0000   1.0000  -0.0690   6.2949   0.0000   0.0000
 1  5 128.7959  56.4134  39.0716   0.0688  -0.4463   1.0000  31.1766   0.4530
      0.1955  -0.3587   6.2148   1.0000  -0.0770   6.6386   1.0000   0.0000
 2  5 128.6090   0.0000   0.0000  -0.5555   0.0000   1.0000   6.0000   0.4721
     10.8735   1.0000   0.0000   1.0000  -0.0242   9.1937   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  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  6 109.1904  70.8314  30.0000   0.2765  -0.3000   1.0000  16.0000   0.1583
      0.2804  -0.1994   8.1117   1.0000  -0.2675   6.2993   0.0000   0.0000
 2  6 137.0000   0.0000   0.0000  -0.1902   0.0000   1.0000   6.0000   0.2256
     17.7186   1.0000   0.0000   1.0000  -0.0377   6.4281   0.0000   0.0000
 3  6 136.6643  41.8662   0.0000   0.2527  -0.3000   1.0000  36.0000   0.6764
      4.9938  -0.3800  10.3140   1.0000  -0.1915   6.2189   1.0000   0.0000
 1  6 125.8776  57.9428   0.0000   0.1077  -0.5558   1.0000  17.2117   0.4687
      0.2379  -0.3297  10.4455   1.0000  -0.1529   6.2959   1.0000   0.0000
 4  6 103.7982  30.4010  20.2000  -0.1419  -0.3025   1.0000  35.5000   0.4217
      0.9927  -0.3060   9.9500   1.0000  -0.1654   8.3456   1.0000   0.0000
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12    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2   0.0464   1.8296   9.9214   1.0029  -1.0000  -1.0000   0.0000
 2  3   0.0403   1.6913  10.4801   0.8774  -1.0000  -1.0000   0.0000
 2  4   0.0524   1.7325  10.1306   0.9982  -1.0000  -1.0000 294.9500
 1  3   0.1028   1.9277   9.1521   1.3399   1.1104   1.1609 631.8500
 1  4   0.2070   1.7366   9.5916   1.2960   1.2008   1.1262 650.0000
 3  4   0.0491   1.7025  10.6101   1.3036   1.1276   1.0173 880.0000
 1  6   0.0937   1.9583  11.0607   1.8627   1.5560  -1.0000 600.0000
 2  6   0.0470   1.6738  11.6877   1.0031  -1.0000  -1.0000   0.0000
 3  6   0.1263   1.6593  10.6833   1.5650   1.4452  -1.0000   0.0000
 4  6   0.1100   1.7548  10.9719   1.7231   1.4584  -1.0000 180.0000
 1  5   0.1408   1.8161   9.9393   1.7986   1.3021   1.4031   0.0000
 2  5   0.0895   1.6239  10.0104   1.4640  -1.0000  -1.0000   0.0000
82    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
 1  1  1  74.0317  32.2712   0.9501   0.0000   0.1780  10.5736   1.0400
 1  1  2  70.6558  14.3658   5.3224   0.0000   0.0058   0.0000   1.0400
 2  1  2  76.7339  14.4217   3.3631   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
 1  1  3  65.1700   8.0170   7.5000   0.0000   0.2028  10.0000   1.0400
 3  1  3  71.7582  26.7070   6.0466   0.0000   0.2000   0.0000   1.8525
 1  1  4  65.4228  43.9870   1.5602   0.0000   0.2000  10.0000   1.8525
 3  1  4  73.7046  23.8131   3.9811   0.0000   0.2000   0.0000   1.8525
 4  1  4  65.6602  40.5852   1.8122   0.0000   0.2000   0.0000   1.8525
 2  1  3  59.4426  17.6020   2.3044   0.0000   0.9699   0.0000   1.1272
 2  1  4  71.0777   9.1462   3.4142   0.0000   0.9110   0.0000   1.0400
 1  2  4   0.0000   0.0019   6.3000   0.0000   0.0000   0.0000   1.0400
 1  3  1  72.1018  38.4720   1.3926   0.0000   0.4785   0.0000   1.2984
 1  3  3  89.9987  44.9806   0.5818   0.0000   0.7472   0.0000   1.2639
 1  3  4  70.3281  13.2989   7.7058   0.0000   0.7472   0.0000   1.2639
 3  3  3  84.2807  24.1938   2.1695 -10.0000   0.7472   0.0000   1.2639
 3  3  4  84.2585  44.1039   0.9185   0.0000   0.7472   0.0000   1.2639
 4  3  4  74.2312  25.7005   4.3943   0.0000   0.7472   0.0000   1.2639
 1  3  2  89.0416  36.9460   0.4569   0.0000   2.7636   0.0000   2.0494
 2  3  3  81.1709   4.2886   6.5904   0.0000   3.0000   0.0000   1.2618
 2  3  4  75.9203  44.9675   0.8889   0.0000   3.0000   0.0000   1.2618
 2  3  2  82.2020  12.7165   3.9296   0.0000   0.2765   0.0000   1.0470
 1  4  1  68.3788  18.3716   1.8893   0.0000   2.4132   0.0000   1.3993
 1  4  3  86.5585  37.6814   1.1611   0.0000   1.7325   0.0000   1.0440
 1  4  4  74.4818  12.0954   7.5000   0.0000   1.7325   0.0000   1.0440
 3  4  3  78.5850  44.3389   1.3239 -19.2266   1.7325  40.0000   1.0440
 3  4  4  77.6245  32.0866   1.8889  -0.9193   1.7325   0.0000   1.0440
 4  4  4  66.4718  15.9087   7.5000   0.0000   1.7325   0.0000   1.0440
 1  4  2  90.0000  33.6636   1.1051   0.0000   0.2638   0.0000   1.1376
 2  4  3  83.8493  44.9000   1.3580   0.0000   0.5355   0.0000   2.5279
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| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 4 | 4 | 78.7452 | 24.2010 | 3.7481 | 0.0000 | 0.5355 | 0.0000 | 2.5279 |
| 2 | 4 | 2 | 55.8679 | 14.2331 | 2.9225 | 0.0000 | 0.2000 | 0.0000 | 2.9932 |
| 1 | 2 | 3 | 0.0000 | 0.0019 | 6.0000 | 0.0000 | 0.0000 | 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 | 0.0019 | 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 | 0.0019 | 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 | 74.4180 | 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 | 85.6645 | 40.0000 | 2.9274 | 0.1463 | 0.5000 | 0.0000 | 1.3830 |
| 2 | 5 | 2 | 83.8555 | 5.1317 | 0.4377 | 0.0000 | 0.5000 | 0.0000 | 3.0000 |
| 2 | 5 | 5 | 97.0064 | 32.1121 | 2.0242 | 0.0000 | 0.5000 | 0.0000 | 2.8568 |
| 6 | 6 | 6 | 69.5456 | 21.6861 | 1.4258 | 0.0000 | -0.2101 | 0.0000 | 1.3241 |
| 2 | 6 | 6 | 75.8168 | 21.6786 | 1.0588 | 0.0000 | 2.5179 | 0.0000 | 1.0400 |
| 2 | 6 | 2 | 78.5939 | 20.9272 | 0.8580 | 0.0000 | 2.8421 | 0.0000 | 1.0400 |
| 3 | 6 | 6 | 70.1016 | 5.3781 | 1.3167 | 0.0000 | 2.1459 | 0.0000 | 1.0400 |
| 2 | 6 | 3 | 73.6706 | 6.7092 | 3.7625 | 0.0000 | 0.8613 | 0.0000 | 1.0400 |
| 3 | 6 | 3 | 90.2344 | 7.7833 | 1.7464 | 0.0000 | 0.7689 | 0.0000 | 1.0400 |
| 6 | 3 | 6 | 25.0715 | 3.6526 | 0.3180 | 0.0000 | 4.1125 | 0.0000 | 1.0400 |
| 3 | 3 | 6 | 73.4663 | 25.0761 | 0.9143 | 0.0000 | 2.2466 | 0.0000 | 1.0400 |
| 2 | 3 | 6 | 63.6634 | 10.0346 | 2.6680 | 0.0000 | 1.6982 | 0.0000 | 1.0400 |
| 1 | 3 | 6 | 53.6634 | 15.7193 | 2.7680 | 0.0000 | 1.6982 | 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 | 6.5625 | 0.0000 | 1.6371 | 0.0000 | 1.0400 |
| 2 | 2 | 5 | 0.0000 | 0.0019 | 6.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0400 |
| 1 | 1 | 6 | 72.5239 | 22.3583 | 2.0393 | 0.0000 | 1.0031 | 0.0000 | 1.0400 |
| 6 | 1 | 6 | 75.3369 | 18.9270 | 2.0703 | 0.0000 | 1.0031 | 0.0000 | 1.0400 |
| 1 | 6 | 1 | 69.3369 | 18.9270 | 2.1333 | 0.0000 | 1.0031 | 0.0000 | 1.0400 |
| 1 | 6 | 3 | 69.3004 | 18.9710 | 2.1533 | 0.0000 | 1.0031 | 0.0000 | 1.0400 |
| 1 | 6 | 6 | 69.3369 | 19.6964 | 2.0703 | 0.0000 | 1.0031 | 0.0000 | 1.0400 |
| 2 | 1 | 6 | 72.5949 | 10.9851 | 1.4246 | 0.0000 | 1.0000 | 0.0000 | 1.0400 |
| 1 | 6 | 2 | 72.5949 | 14.8347 | 2.4952 | 0.0000 | 1.0000 | 0.0000 | 1.0400 |
| 4 | 6 | 6 | 0.0000 | 30.0000 | 6.0000 | 0.0000 | 1.0000 | 0.0000 | 1.0400 |
| 4 | 6 | 4 | 74.2811 | 10.5525 | 2.0350 | 0.0000 | 0.9925 | 0.0000 | 1.0693 |
| 3 | 6 | 4 | 77.5533 | 10.2000 | 2.0100 | 0.0000 | 0.9900 | 0.0000 | 1.0500 |
| 6 | 4 | 6 | 76.5000 | 10.2000 | 2.0200 | 0.0000 | 1.0050 | 0.0000 | 1.0300 |
| 2 | 6 | 4 | 70.5000 | 10.0357 | 1.2043 | 0.0000 | 1.0151 | 0.0000 | 1.0388 |
| 2 | 4 | 6 | 70.5000 | 10.0250 | 2.0067 | 0.0000 | 1.0050 | 0.0000 | 1.0500 |
| 4 | 4 | 6 | 77.5000 | 10.2055 | 2.0200 | 0.0000 | 0.9900 | 0.0000 | 1.0400 |
| 3 | 4 | 6 | 77.0000 | 10.0000 | 2.0000 | 0.0000 | 1.0000 | 0.0000 | 1.0400 |

```
 4  3  6  77.0000  10.0000   2.0000   0.0000   1.0000   0.0000   1.0400
 4  2  6   0.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0400
 3  1  6  71.5949  10.8121   2.5256   0.0000   1.0000   0.0000   1.0400
 1  2  6   0.0000  10.0000   2.0000   0.0000   1.0000   0.0000   1.0400
35    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1  1  1  1   0.0000  48.4194   0.3163  -8.6506  -1.7255   0.0000   0.0000
 1  1  1  2   0.0000  63.3484   0.2210  -8.8401  -1.8081   0.0000   0.0000
 2  1  1  2   0.0000  45.2741   0.4171  -6.9800  -1.2359   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  1  3  0   1.7254  86.0769   0.3440  -4.2330  -2.0000   0.0000   0.0000
 0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  3  3  0   1.2314 116.5137   0.5599  -4.1412   0.0000   0.0000   0.0000
 0  1  4  0  -1.3258 149.8644   0.4790  -7.1541  -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   1.3168  57.0732   0.2679  -4.1516  -2.0000   0.0000   0.0000
 0  4  4  0   2.0000  75.3685  -0.7852  -9.0000  -2.0000   0.0000   0.0000
 0  1  1  0   0.0930  18.6070  -1.3191  -9.0000  -1.0000   0.0000   0.0000
 4  1  4  4  -2.0000  20.6655  -1.5000  -9.0000  -2.0000   0.0000   0.0000
 0  1  5  0   4.0885  78.7058   0.1174  -2.1639   0.0000   0.0000   0.0000
 0  5  5  0  -0.0170 -56.0786   0.6132  -2.2092   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
 0  4  6  0   0.0000   0.0000   0.0000  -2.4426   0.0000   0.0000   0.0000
 1  1  3  3   1.2707  21.6200   1.5000  -9.0000  -2.0000   0.0000   0.0000
 1  3  3  1  -1.8804  79.9255  -1.5000  -4.1940  -2.0000   0.0000   0.0000
 3  1  3  3  -2.0000  22.5092   1.5000  -8.9500  -2.0000   0.0000   0.0000
 1  4  4  3   0.1040  70.1152   0.5284  -3.5026  -2.0000   0.0000   0.0000
 1  1  3  4   1.2181 119.6186  -1.5000  -7.0635  -2.0000   0.0000   0.0000
 2  1  3  4  -2.0000 156.6604   1.1004  -7.3729  -2.0000   0.0000   0.0000
 1  3  4  3   2.0000  96.6281  -1.5000  -3.8076  -2.0000   0.0000   0.0000
 1  1  4  2  -2.0000 147.2445  -1.5000  -7.0142  -2.0000   0.0000   0.0000
 1  1  4  3  -2.0000  47.8326  -1.5000  -9.0000  -2.0000   0.0000   0.0000
 2  3  4  3  -0.2997 152.9040  -1.5000  -4.4564  -2.0000   0.0000   0.0000
 2  4  4  3   0.1040  70.1152   0.5284  -3.5026  -2.0000   0.0000   0.0000
 6  1  3  4   2.0000  70.2461   2.0000  -3.0635  -2.0000   0.0000   0.0000
 3  1  6  1   5.0000  80.6070   5.0000  -3.0000  -2.0000   0.0000   0.0000
 1  3  6  1   1.0000  80.6070   1.0000  -3.0000  -2.0000   0.0000   0.0000
 9  ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
 3  2  3   2.1845  -2.3549   3.0582  19.1627
 3  2  4   1.7058  -3.8907   3.0582  19.1627
 4  2  3   1.8738  -3.5421   3.0582  19.1627
 4  2  4   1.8075  -4.1846   3.0582  19.1627
 3  2  5   2.6644  -3.0000   3.0000   3.0000
```

| | | | | | | |
|---|---|---|---|---|---|---|
| 4 | 2 | 5 | 4.0476 | -3.0000 | 3.0000 | 3.0000 |
| 5 | 2 | 3 | 2.1126 | -4.5790 | 3.0000 | 3.0000 |
| 5 | 2 | 4 | 2.2066 | -5.7038 | 3.0000 | 3.0000 |
| 5 | 2 | 5 | 1.9461 | -4.0000 | 3.0000 | 3.0000 |

**Table S1.** Bond order cut-off values for various atom pairs. *BondFrag* program uses these values to determine molecular fragments.

| | **C** | **H** | **O** | **N** | **Si** |
|---|---|---|---|---|---|
| **C** | 0.55 | 0.40 | 0.80 | 0.30 | 0.3 |
| **H** | | 0.55 | 0.40 | 0.55 | 0.3 |
| **O** | | | 0.65 | 0.55 | 0.75 |
| **N** | | | | 0.45 | 0.3 |
| **Si** | | | | | 0.3 |

**Figure S1**

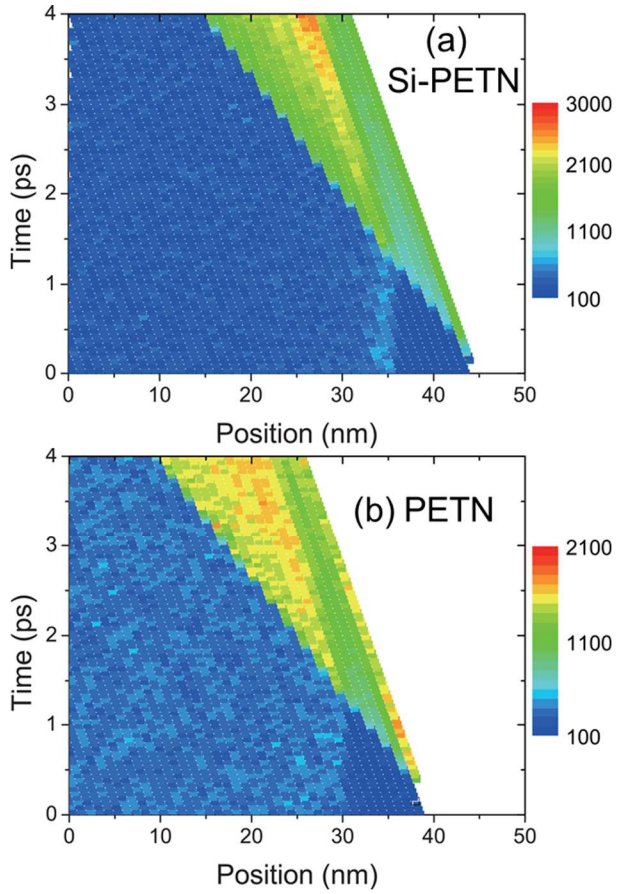


Figure S1. Temperature−Time−Position diagram for the shock met the first convex polymer asperity from polymer to EM with $U_p$ = 3.5 km/s. (a) The hotspot forms and its temperature increases for Si-PETN. (b) The hotspot forms and remains at a constant temperature for some finite amount of time (3 ps) for PETN.

**Figure S2**

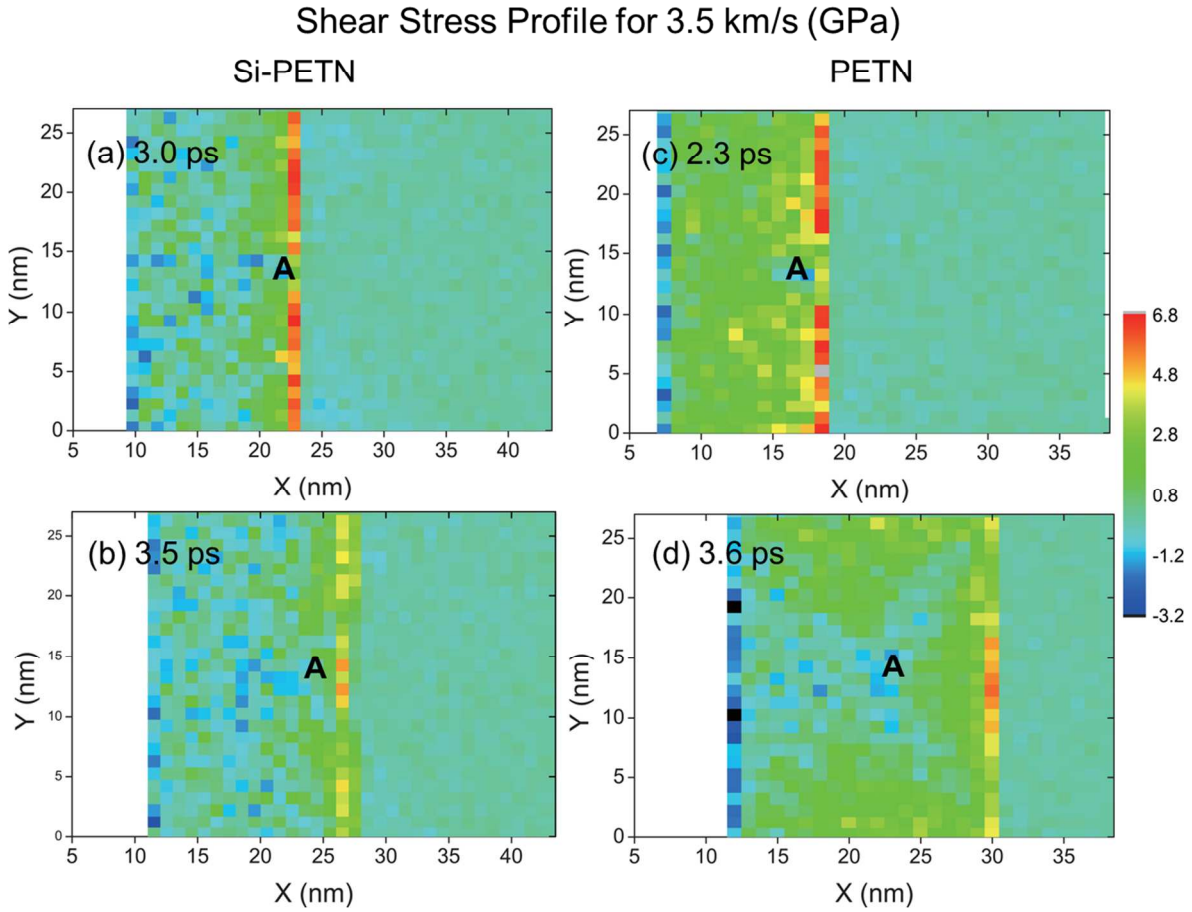


**Figure S2:** 2-dimensional shear stress profiles of Si-PETN (a-b) and PETN (c-d) with $U_p$ = 3.5 km/s. The local shear stress relaxation caused the hotspot formation (marked as A) for both Si-PETN and PETN.

**Figure S3**

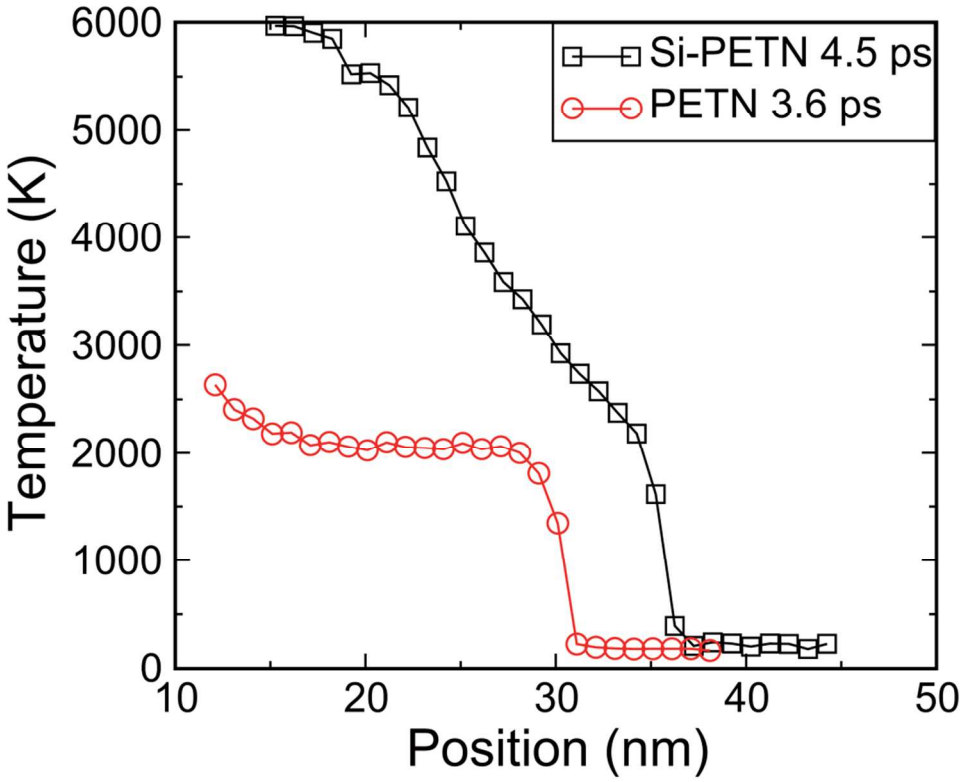


Figure S3. One dimensional temperature profiles for Si-PETN and PETN as shocks encounter the second (concave) polymer asperity region from explosives to polymer with $U_p$ = 3.5 km/s.

**Figure S4**

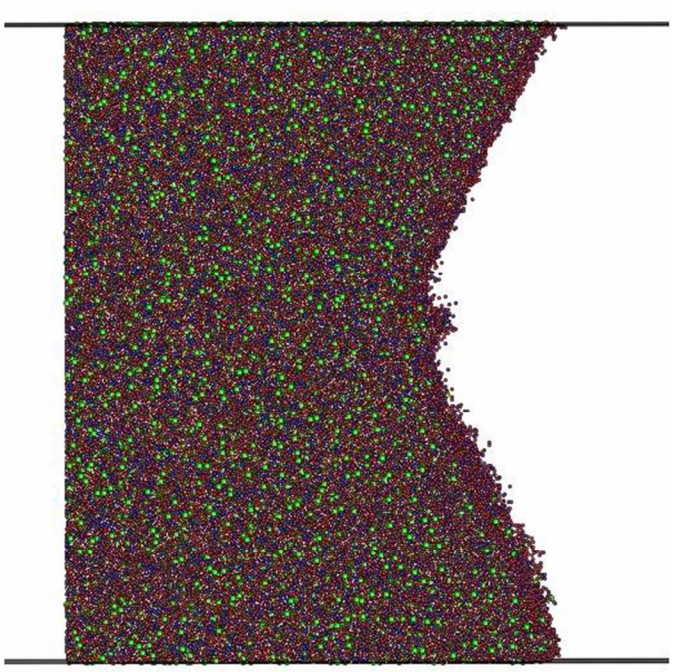

Figure S4. The initiation of interfacial instability of Si-PETN due to the dramatically chemical reactions. Shock moves from Si-PETN to polymer with $U_p$ = 3.5 km/s.