Electronic supplementary information (ESI) for

ReaxFF Molecular Dynamics Simulations on Lithiated Sulfur Cathode Materials

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CONTENTS

Li-S force field parameters

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Reactive MD-force field: Li/S PCCP 2014
 39       ! Number of general parameters
   50.0000 !p(boc1)
    9.5469 !p(boc2)
   26.5405 !p(coa2)
    1.5105 !p(trip4)
    6.6630 !p(trip3)
   70.0000 !kc2
    1.0588 !p(ovun6)
    4.6000 !p(trip2)
   12.1176 !p(ovun7)
   13.3056 !p(ovun8)
  -10.1292 !p(trip1)
    0.0000 !Lower Taper-radius (swa)
   10.0000 !Upper Taper-radius (swb)
    0.0000 !not used
   33.8667 !p(val7)
    6.0891 !p(lp1)
    1.0563 !p(val9)
    2.0384 !p(val10)
    6.1431 !not used
    6.9290 !p(pen2)
    0.3989 !p(pen3)
    3.9954 !p(pen4)
    0.0000 !not used
    5.7796 !p(tor2)
   10.0000 !p(tor3)
    1.9487 !p(tor4)
    0.0000 !not used
    2.1645 !p(cot2)
    1.5591 !p(vdW1)
    0.1000 !Cutoff for bond order*100 (cutoff)
    2.1365 !p(coa4)
    0.6991 !p(ovun4)
   50.0000 !p(ovun3)
    1.8512 !p(val8)
    0.0000 !not used
    0.0000 !not used
    0.0000 !not used
    0.0000 !not used
    2.6962 !p(coa3)
  2    ! Nr of atoms; atomID;ro(sigma); Val;atom mass;Rvdw;Dij;gamma
           alfa;gamma(w);Val(angle);p(ovun5);n.u.;chiEEM;etaEEM;n.u.
           ro(pipi);p(lp2);Heat increment;p(boc4);p(boc3);p(boc5),n.u.;n.u.
           p(ovun2);p(val3);n.u.;Val(boc);p(val5);n.u.;n.u.;n.u.
 S    1.9186   2.0000  32.0600   1.6516   0.4937   0.7530   1.6593   6.0000
      9.0227   4.9055   4.0000  30.0000 112.1416   6.5745   9.0000   2.0000
      1.0000   3.4994  65.0000  12.0000  22.1978  15.3230   0.9745   0.0000
    -15.7363   2.8802   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
 Li   1.9814   1.0000   6.9410   1.8000   0.2939   0.9387  -0.1000   1.0000
      9.0616   1.3258   1.0000   0.0000   0.0000  -3.0000  10.0241   0.0000
     -1.0000   0.0000  37.5000   5.4409   6.9107   0.1973   0.8563   0.0000
     -2.5068   2.2989   1.0338   1.0000   2.8103   1.3000   0.2000  13.0000
  3      ! Nr of bonds; at1;at2;De(sigma);De(pi);De(pipi);p(be1);p(b
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                    p(be2);p(bo3);p(bo4);n.u.;p(bo1);p(bo2)
1   1   84.3765   31.1563    0.0000   -0.8610   -0.4781    1.0000   17.8574    0.3198
         0.4942   -0.1773    8.4125    1.0000   -0.0889    6.8515    1.0000    0.0000
1   2   68.4187    0.0000    0.0000   -0.3842   -0.5000    0.0000   25.0000    0.2561
         0.4468   -0.2500   20.0000    1.0000   -0.1990    6.0316    0.0000    0.0000
2   2   34.3154    0.0000    0.0000    0.5995    0.3000    0.0000   26.0000    0.5445
         0.5752    0.0000   12.0000    1.0000   -0.1382    4.5000    0.0000    0.0000
1     ! Nr of off-diagonal terms. at1;at2;Dij;RvdW;alfa;ro(sigma);r
1   2    0.2114    2.0191   10.2498    2.0765   -1.0000   -1.0000
5     ! Nr of angles. at1;at2;at3;Thetao,o;p(val1);p(val2);p(coa1);
1   1   1   70.3671    5.7180    7.0000    0.0000    0.3683    0.0000    2.4869
1   2   1   66.4795    8.0479    5.0000    0.0000    1.3950    0.0000    1.6004
2   1   2   75.6682    7.4119    3.8037    0.0000    0.0100    0.0000    3.4502
1   1   2  100.0000    5.2297    0.8528    0.0000    1.0382    0.0000    1.1870
1   2   2   78.8126    1.9499    3.4361    0.0000    0.0100    0.0000    3.6457
3     ! Nr of torsions. at1;at2;at3;at4;;V1;V2;V3;p(tor1);p(cot1);n
1   1   1   1    1.8235  -11.0688   -0.4137   -2.7875    0.0000    0.0000    0.0000
1   1   1   2    0.0000    2.0000    0.0100   -9.0000    0.0000    0.0000    0.0000
2   1   1   2    0.0000   20.0000    0.0100   -5.0000    0.0000    0.0000    0.0000
0     ! Nr of hydrogen bonds. at1;at2;at3;r(hb);p(hb1);p(hb2);p(hb3
```

Stress-strain diagram for the strain rate of $5x10^8$ (s^{-1}) and $1x10^8$ (s^{-1})

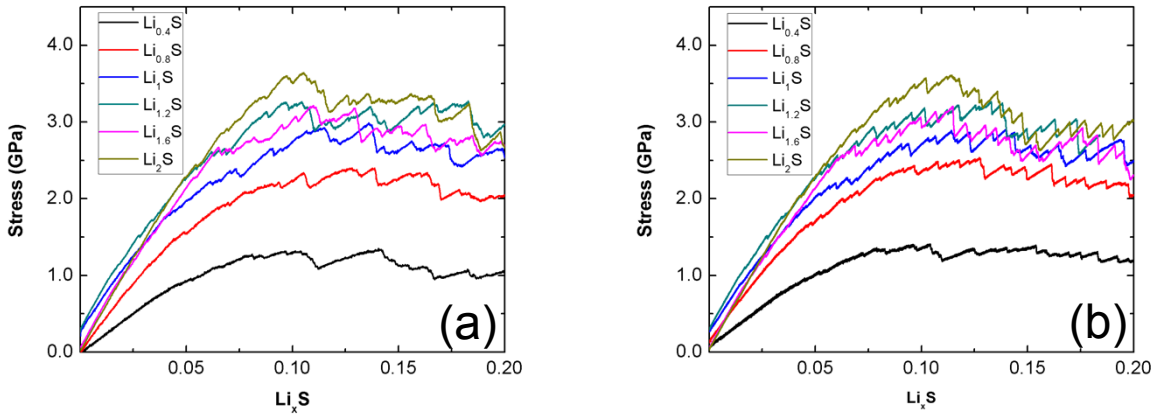

Fig S1: Stress-strain curve for the a-Li_xS compositions at the strain rate of (a) $5x10^8$ s^{-1}, and (b) $1x10^8$ s^{-1}