Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary information for:

Binding is responsible for exceptional hardness in Polyethylene/silicalite nanocomposite materi-als.

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Here the geometries of before and after relaxation of PE strains are reported, in the format of CRYSTAL input, as well as the basis set of Gaussian functions used in the calculations. In Figure S1 additional views of the PE structures before and after relaxation of the strains are depicted, as a complement to Figure 2 of the manuscript.

Optimized Geometry of Structure (before relaxation)

```
CRYSTAL
0 0 0
62
 20.16166799    19.65200771    13.70924045
69
14    4.287326996272E-01  5.578704723638E-02 -3.459180853111E-01
14    3.118037986812E-01  3.153783244293E-02 -2.013886539783E-01
14    2.834697531786E-01  6.566583887358E-02  1.805828541692E-02
14    1.247359641619E-01  6.819040559957E-02  2.338910761888E-02
14    7.774151502169E-02  3.201420265895E-02 -1.877844922583E-01
14    1.862823090048E-01  5.573844065088E-02 -3.420360897684E-01
14    4.245133806200E-01 -1.714963598341E-01 -3.248346797111E-01
14    3.078527058612E-01 -1.273540915058E-01 -1.896237069381E-01
14    2.611293765948E-01 -1.699499952795E-01  2.285558844100E-02
14    1.105615836847E-01 -1.716381395408E-01  1.820365380420E-02
14    6.986489648042E-02 -1.266515793249E-01 -1.894851659233E-01
14    1.866232705609E-01 -1.699876004230E-01 -3.234417590134E-01
8     4.994070847904E-01  4.394634054673E-02 -2.926155376763E-01
8     3.721162698408E-01  6.546233424162E-02 -2.628653860156E-01
8     4.346834445547E-01  1.240588399073E-01 -4.121817675837E-01
8     4.131918275435E-01 -7.649522728351E-03 -4.184559932727E-01
8     3.034803405660E-01  6.910549543943E-02 -9.658769044944E-02
8     3.286214239742E-01 -4.797117549153E-02 -1.819572636809E-01
8     2.440602589082E-01  3.746714907677E-02 -2.640602702582E-01
8     3.081160979142E-01  1.360457807802E-01  6.868057940021E-02
8     2.039473864650E-01  5.509413315944E-02  2.991836148514E-02
8     3.187531969559E-01  1.784716126809E-03  7.289668745397E-02
8     1.058938430311E-01  1.399084574836E-01  7.502149221276E-02
8     1.012857558623E-01  7.142859777238E-02 -8.950082763467E-02
8     1.170847096329E-01  6.053610344061E-02 -2.823482856829E-01
8     9.363141144387E-02 -4.854099596977E-02 -1.727951035242E-01
8     1.991047064616E-01  1.286673242174E-01 -3.936597896898E-01
8     4.903442419037E-01 -1.296396148590E-01 -2.910891523518E-01
8     3.684697269683E-01 -1.683889529292E-01 -2.399622859981E-01
8     4.445862296820E-01 -2.500000000000E-01 -3.440814464289E-01
8     2.947207247003E-01 -1.593889982474E-01 -8.306705875590E-02
8     2.402448339078E-01 -1.326526959765E-01 -2.530808454810E-01
8     2.599839627917E-01 -2.500000000000E-01  5.003379515042E-02
8     1.856111066388E-01 -1.409876105594E-01  2.049036073207E-02
8     1.089314305926E-01 -2.500000000000E-01  5.326326541021E-02
8     8.351806179692E-02 -1.705690643012E-01 -9.219495764773E-02
8     1.132072032650E-01 -1.603481176828E-01 -2.769691694105E-01
8     2.044205713610E-01 -2.500000000000E-01 -3.322317612929E-01
6     3.055176314370E-01 -2.500000000000E-01  3.566354044138E-01
6    -3.812505416919E-01 -2.500000000000E-01  2.347482282247E-01
6     4.194339004438E-01 -2.500000000000E-01 -1.791839216775E-02
6    -4.667276249152E-02 -1.819659362745E-01  4.960902889472E-01
6    -3.496349216269E-01  2.500000000000E-01 -2.638812795787E-01
6     4.454557190360E-03 -8.158487846558E-02 -4.189426848192E-01
6    -2.640632351710E-01 -2.500000000000E-01  1.925262514943E-01
6     7.496276066141E-02  2.500000000000E-01 -2.628942916994E-01
6    -4.551502346166E-01 -2.500000000000E-01  2.118754340669E-01
6     4.907611088450E-01 -2.500000000000E-01  2.938544787685E-01
6     9.868749411646E-03 -1.585091087465E-01 -4.374808403915E-01
6     1.031019303665E-02 -3.686088640166E-02  4.901295387860E-01
6    -3.333236945148E-01 -2.500000000000E-01  1.461292815760E-01
1     4.953521187617E-01 -2.052089616612E-01  3.404498832049E-01
1    -4.645226223233E-01 -2.943079853165E-01  1.654258594949E-01
1    -3.687998481887E-01 -2.055133785586E-01  2.789674720955E-01
1    -3.414330613975E-01 -2.949214770541E-01  1.002563069430E-01
1    -2.637578695826E-01 -2.059592482328E-01  2.417916853611E-01
1    -1.869162645101E-01 -2.949741504826E-01  9.724917351363E-02
1    -1.689665457110E-01 -2.935246726856E-01  2.767816379214E-01
1    -7.091152830540E-02 -2.939584331790E-01  3.109045129079E-01
1     4.026230674814E-01 -2.500000000000E-01 -9.387006336970E-02
1     3.745622219979E-01 -2.500000000000E-01  2.632850071213E-02
1    -8.554925080018E-02 -1.432915699127E-01  4.993390670830E-01
1    -2.993996703155E-02 -1.806885375461E-01  4.208077676708E-01
1    -4.587493190717E-01 -6.376593467296E-02 -1.337167343382E-01
1     4.562600632793E-01 -7.185909690343E-02 -1.155075100785E-01
1     5.826151627791E-02 -1.712164462061E-01 -4.691025018724E-01
1     7.256780332655E-03 -1.857400147120E-01 -3.682963621896E-01
1     6.170794763274E-02 -4.621343696536E-01  4.635833536789E-01
1    -1.964112932163E-02 -4.425279690615E-01  4.304603743538E-01
```

Optimized Geometry of Structure (after relaxation)

CRYSTAL
0 0 0
62
19.99774509 19.74748922 13.66426915
69
 14 4.291858532232E-01 5.474905216623E-02 -3.486367276649E-01
 14 3.099514515510E-01 3.327559806332E-02 -2.065430798278E-01
 14 2.850218953831E-01 6.906723759541E-02 1.334695366370E-02
 14 1.254505934289E-01 6.827328030697E-02 1.933711846806E-02
 14 7.931686928627E-02 2.732178905697E-02 -1.913178432495E-01
 14 1.838627031870E-01 5.436479069042E-02 -3.513471938596E-01
 14 4.247293026914E-01 -1.711298425039E-01 -3.301883842868E-01
 14 3.045452418920E-01 -1.243926158131E-01 -1.973234809136E-01
 14 2.636574958676E-01 -1.702290522531E-01 1.843782285857E-02
 14 1.111133280417E-01 -1.725978619794E-01 2.267085762712E-02
 14 7.184181924002E-02 -1.305627758436E-01 -1.889954812957E-01
 14 1.857673343460E-01 -1.713397934045E-01 -3.296683322154E-01
  8 4.997274777917E-01 3.851028803800E-02 -2.962232293645E-01
  8 3.733593867515E-01 6.521685833482E-02 -2.640708908602E-01
  8 4.366077284278E-01 1.237110646973E-01 -4.126745344424E-01
  8 4.105021572979E-01 -6.139337285460E-03 -4.236078610035E-01
  8 2.994797918227E-01 7.240309053021E-02 -1.033083443357E-01
  8 3.247764704228E-01 -4.576891131946E-02 -1.821806426460E-01
  8 2.442918497370E-01 4.006748173264E-02 -2.749671436409E-01
  8 3.147754107980E-01 1.383002469917E-01 6.132029351852E-02
  8 2.054125096593E-01 6.211773775772E-02 3.415580208515E-02
  8 3.201199743128E-01 3.819139785129E-03 6.455865592499E-02
  8 9.902325090735E-02 1.388251829241E-01 6.606665869544E-02
  8 1.072095169089E-01 6.737102530706E-02 -9.592121895787E-02
  8 1.148500340361E-01 5.592968830758E-02 -2.893077018032E-01
  8 9.643495526084E-02 -5.263911891668E-02 -1.765970901200E-01
  8 1.912972397723E-01 1.269319035228E-01 -4.058278273914E-01
  8 4.918443811714E-01 -1.333063187241E-01 -2.907437679193E-01
  8 3.658183681533E-01 -1.636645106404E-01 -2.495667278951E-01
  8 4.413331059234E-01 -2.499999999996E-01 -3.489376650475E-01
  8 2.869410444408E-01 -1.597515702466E-01 -9.398576649000E-02
  8 2.385118053475E-01 -1.275396589165E-01 -2.655481228393E-01
  8 2.683897553249E-01 -2.499999999996E-01 4.476759801446E-02
  8 1.870738856227E-01 -1.433336241536E-01 2.977565395209E-02
  8 1.082753364959E-01 -2.499999999996E-01 6.134273463064E-02
  8 8.713371978562E-02 -1.725163067582E-01 -9.002210178728E-02
  8 1.133888221185E-01 -1.665125164524E-01 -2.767689840822E-01
  8 2.088636546144E-01 -2.499999999996E-01 -3.363848067759E-01
  6 -4.934278514503E-01 -2.499999999996E-01 2.683614676031E-01
  6 -1.916858597644E-01 -2.499999999996E-01 2.218913184938E-01
  6 4.222880618771E-01 -2.499999999996E-01 -7.322673589090E-02
  6 -5.652886614184E-02 -1.827213661906E-01 -4.735953552670E-01
  6 4.567551299317E-01 2.499999999996E-01 -1.687862968800E-01
  6 1.738867707811E-02 -8.273601388690E-02 -4.256791485294E-01
  6 -6.910943945149E-02 -2.499999999996E-01 2.549450059829E-01
  6 -1.199922913697E-01 2.499999999996E-01 -3.562462510120E-01
  6 -2.543550220232E-01 -2.499999999996E-01 1.574432236589E-01
  6 -3.210897248708E-01 -2.499999999996E-01 2.159868590170E-01
  6 1.440967743775E-02 -1.588528577991E-01 -4.475114940861E-01
  6 3.198345349413E-03 -3.740311644785E-02 4.860880394968E-01
  6 -1.220075834224E-01 -2.499999999996E-01 1.727866494351E-01
  1 -3.228924550983E-01 -2.055046659714E-01 2.641145876782E-01
  1 -2.538472163765E-01 -2.942909210880E-01 1.088633379212E-01
  1 -1.939134176822E-01 -2.059582391065E-01 2.703325515120E-01
  1 -1.160780396040E-01 -2.945308830654E-01 1.254954709551E-01
  1 -7.954305201316E-02 -2.058102673212E-01 3.012944158410E-01
  1 1.908645738566E-02 -2.944474944551E-01 1.881679859387E-01
  1 2.273793852691E-02 -2.936377121127E-01 3.697608042223E-01
  1 1.283526917377E-01 -2.938478251859E-01 4.038961462241E-01
  1 4.400868333819E-01 -2.499999999996E-01 -1.488932741704E-01
  1 3.681484890080E-01 -2.499999999996E-01 -7.931770018932E-02
  1 -9.093656236502E-02 -1.438183113312E-01 -4.468623580619E-01
  1 -6.450169103904E-02 -1.842002151944E-01 4.473348605082E-01
  1 -4.334984148501E-01 -6.920427726023E-02 -1.038996940850E-01
  1 4.809241714657E-01 -7.099857665198E-02 -1.318907178941E-01
  1 5.047261325668E-02 -1.712196323731E-01 4.951588630728E-01
  1 3.082818992459E-02 -1.868321427860E-01 -3.832773421493E-01
  1 4.313018374418E-02 -4.564127313599E-01 4.314258785832E-01
  1 -4.279752846402E-02 -4.461414712589E-01 4.496393873756E-01

Basis Set

14 5

```
0 0 8 2.0 1.0
 149866.0 0.0001215
 22080.6 0.0009770
 4817.5 0.0055181
 1273.5 0.0252000
 385.11 0.0926563
 128.429 0.2608729
 45.4475 0.4637538
 16.2589 0.2952000
0 1 8 8.0 1.0
 881.111 -0.0003 0.0006809
 205.84 -0.0050 0.0059446
 64.8552 -0.0368 0.0312000
 23.9 -0.1079 0.1084000
 10.001 0.0134 0.2378000
 4.4722 0.3675 0.3560066
 2.034 0.5685 0.3410000
 0.9079 0.2065 0.1326000
0 1 3 4.0 1.0
 2.6668 -0.0491 0.0465000
 1.0780 -0.1167 -0.1005000
 0.3682 0.2300 -1.0329000
0 1 1 0.0 1.0
 0.193 1.0 1.0
0 3 1 0. 1.
 0.610 1.0
8 5
0 0 8 2.0 1.0
 8020.0 0.00108
 1338.0 0.00804
 255.4 0.05324
 69.22 0.1681
 23.90 0.3581
 9.264 0.3855
 3.851 0.1468
 1.212 0.0728
0 1 4 6.0 1.0
 49.43 -0.00883 0.00958
 10.47 -0.0915 0.0696
 3.235 -0.0402 0.2065
 1.217 0.379 0.347
0 1 1 0.0 1.0
 0.500 1.0 1.0
0 1 1 0.0 1.0
 0.191 1.0 1.0
0 3 1 0.0 1.0
 0.500 1.0
6 4
0 0 6 2.0 1.0
 .3047524880D+04 .1834737130D-02
 .4573695180D+03 .1403732280D-01
 .1039486850D+03 .6884262220D-01
 .2921015530D+02 .2321844430D+00
 .9286662960D+01 .4679413480D+00
 .3163926960D+01 .3623119850D+00
0 1 3 4.0 1.0
 .7868272350D+01 -.1193324200D+00 .6899906660D-01
 .1881288540D+01 -.1608541520D+00 .3164239610D+00
 .5442492580D+00 .1143456440D+01 .7443082910D+00
0 1 1 0.0 1.0
 .1687144782D+00 .1000000000D+01 .1000000000D+01
0 3 1 0.0 1.0
 .8000000000D+00 .1000000000D+01
1 3
0 0 3 1. 1.
 0.1873113696D+02 0.3349460434D-01
 0.2825394365D+01 0.2347269535D+00
 0.6401216923D+00 0.8137573261D+00
0 0 1 0. 1.
 0.1612777588D+00 0.1000000000D+01
0 2 1 0. 1.
 0.1100000000D+01 0.1000000000D+01
```

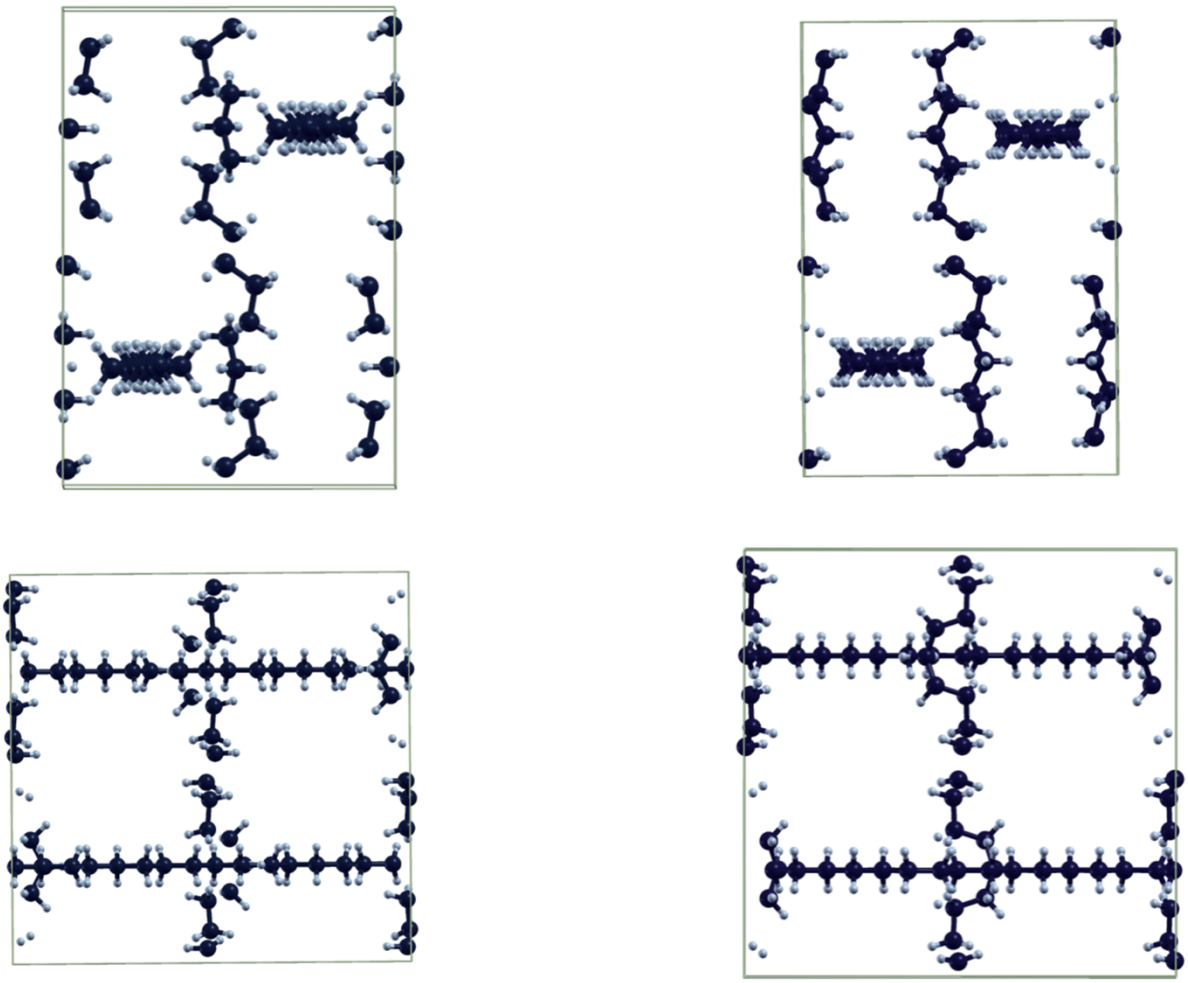

Figure S 1: Other views of Polyethylene chains. Complementary to Figure 2 in the manuscript, here additional views of unrelaxed (left panels) and relaxed (right panels) structure of PE are shown.