

Supporting Information

Solid-state order and charge mobility in [5]-[12] cycloparaphenylenes

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S1. DFT optimized Cartesian coordinates.

S2. Representative MD snapshots of [n]CPPs equilibrated at 300K.

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Table S2. MD equilibrated supercell parameters.

Table S3. Strain per phenyl ring found from B3LYP/6-311G(d,p).

S1. DFT optimized Cartesian coordinates

[5]CPP:

```
50
00000001
C      1.682000    2.741000    1.293000
H      1.123000    2.890000    2.208000
C      2.698000    1.795000    1.305000
H      2.874000    1.264000    2.232000
C      3.282000    1.338000    0.110000
C      3.551000   -0.127000   -0.018000
C      3.544000   -0.984000    1.101000
H      3.894000   -0.625000    2.063000
C      2.928000   -2.227000    1.053000
H      2.824000   -2.779000    1.979000
C      2.276000   -2.671000   -0.116000
C      0.961000   -3.375000   -0.053000
C      0.155000   -3.517000   -1.199000
H      0.609000   -3.614000   -2.178000
C     -1.218000   -3.316000   -1.137000
H     -1.759000   -3.251000   -2.073000
C     -1.852000   -2.983000    0.076000
C     -0.852000    3.104000   -1.282000
H     -0.268000    3.105000   -2.194000
C     -2.084000    2.467000   -1.308000
H     -2.391000    2.011000   -2.241000
C     -2.778000    2.176000   -0.120000
C     -3.445000    0.844000   -0.005000
C     -3.647000    0.022000   -1.132000
H     -3.853000    0.464000   -2.100000
C     -3.392000   -1.342000   -1.078000
H     -3.402000   -1.897000   -2.009000
C     -2.928000   -1.949000    0.107000
C     -3.144000   -1.201000    1.280000
H     -2.928000   -1.631000    2.250000
C     -3.389000    0.164000    1.225000
H     -3.334000    0.722000    2.152000
C      0.269000   -3.452000    1.172000
H      0.816000   -3.473000    2.107000
C     -1.105000   -3.273000    1.234000
H     -1.556000   -3.181000    2.215000
C      1.212000    3.288000    0.086000
C      2.064000    3.121000   -1.024000
H      1.849000    3.632000   -1.956000
C      3.067000    2.161000   -1.015000
H      3.594000    1.962000   -1.942000
C     -0.259000    3.492000   -0.068000
C     -1.131000    3.553000    1.038000
H     -0.792000    3.978000    1.976000
C     -2.360000    2.905000    1.013000
H     -2.929000    2.851000    1.935000
C      3.261000   -0.750000   -1.246000
H      3.326000   -0.187000   -2.168000
C      2.639000   -1.991000   -1.293000
```

H	2.264000	-2.324000	-2.253000
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[6]CPP:

60

00000001

C	3.166000	-2.743000	0.072000
C	4.188000	-0.093000	0.072000
C	3.763000	-0.708000	1.262000
H	3.635000	-0.112000	2.158000
C	3.264000	-2.003000	1.262000
H	2.771000	-2.359000	2.158000
C	3.887000	-2.244000	-1.030000
H	3.957000	-2.830000	-1.940000
C	4.388000	-0.947000	-1.030000
H	4.833000	-0.560000	-1.939000
C	3.959000	1.370000	-0.072000
C	2.175000	3.580000	-0.072000
C	2.494000	2.905000	-1.262000
H	1.915000	3.092000	-2.158000
C	3.366000	1.825000	-1.262000
H	3.428000	1.220000	-2.158000
C	3.887000	2.244000	1.030000
H	4.430000	2.012000	1.940000
C	3.014000	3.326000	1.030000
H	2.901000	3.906000	1.939000
C	-0.793000	-4.114000	-0.072000
C	2.013000	-3.673000	-0.072000
C	1.268000	-3.612000	-1.262000
H	1.720000	-3.204000	-2.158000
C	-0.103000	-3.828000	-1.262000
H	-0.658000	-3.579000	-2.158000
C	0.000000	-4.488000	1.030000
H	-0.472000	-4.842000	1.940000
C	1.373000	-4.274000	1.030000
H	1.932000	-4.466000	1.939000
C	-3.959000	-1.370000	0.072000
C	-2.175000	-3.580000	0.072000
C	-2.494000	-2.905000	1.262000
H	-1.915000	-3.092000	2.158000
C	-3.366000	-1.825000	1.262000
H	-3.428000	-1.220000	2.158000
C	-3.887000	-2.244000	-1.030000
H	-4.430000	-2.012000	-1.940000
C	-3.014000	-3.326000	-1.030000
H	-2.901000	-3.906000	-1.939000
C	0.793000	4.114000	0.072000
C	-2.013000	3.673000	0.072000
C	-1.268000	3.612000	1.262000
H	-1.720000	3.204000	2.158000
C	0.103000	3.828000	1.262000
H	0.658000	3.579000	2.158000
C	0.000000	4.488000	-1.030000
H	0.472000	4.842000	-1.940000
C	-1.373000	4.274000	-1.030000
H	-1.932000	4.466000	-1.939000

C	-3.166000	2.743000	-0.072000
C	-4.188000	0.093000	-0.072000
C	-3.763000	0.708000	-1.262000
H	-3.635000	0.112000	-2.158000
C	-3.264000	2.003000	-1.262000
H	-2.771000	2.359000	-2.158000
C	-3.887000	2.244000	1.030000
H	-3.957000	2.830000	1.940000
C	-4.388000	0.947000	1.030000
H	-4.833000	0.560000	1.939000

[7]CPP:

70

00000001

C	-1.200000	-4.485000	0.694000
H	-2.100000	-4.169000	1.207000
C	1.262000	-3.295000	3.049000
H	2.160000	-3.465000	2.468000
C	-0.154000	2.416000	4.214000
C	-1.047000	-2.689000	4.443000
H	-1.961000	-2.475000	4.986000
C	0.165000	4.823000	0.745000
C	1.316000	4.450000	1.461000
H	2.291000	4.499000	0.995000
C	0.936000	1.835000	4.889000
H	1.823000	2.426000	5.093000
C	1.234000	-2.210000	3.914000
H	2.110000	-1.576000	3.973000
C	0.953000	0.479000	5.195000
H	1.852000	0.049000	5.624000
C	-0.013000	-4.668000	1.421000
C	-1.034000	4.833000	1.485000
H	-1.947000	5.206000	1.038000
C	1.104000	-5.119000	0.695000
H	2.017000	-5.381000	1.219000
C	0.097000	-4.022000	2.756000
C	-0.123000	-0.357000	4.847000
C	0.039000	-1.799000	4.525000
C	-1.119000	4.237000	2.736000
H	-2.088000	4.184000	3.219000
C	-0.012000	3.587000	3.311000
C	-1.018000	-3.777000	3.578000
H	-1.910000	-4.385000	3.471000
C	1.230000	3.839000	2.703000
H	2.133000	3.418000	3.128000
C	-1.316000	1.633000	4.120000
H	-2.199000	2.036000	3.640000
C	-1.302000	0.281000	4.430000
H	-2.172000	-0.313000	4.179000
C	-1.200000	-4.485000	-0.694000
H	-2.100000	-4.169000	-1.207000
C	1.262000	-3.295000	-3.049000
H	2.160000	-3.465000	-2.468000
C	-0.154000	2.416000	-4.214000

C	-1.047000	-2.689000	-4.443000
H	-1.961000	-2.475000	-4.986000
C	0.165000	4.823000	-0.745000
C	1.316000	4.450000	-1.461000
H	2.291000	4.499000	-0.995000
C	0.936000	1.835000	-4.889000
H	1.823000	2.426000	-5.093000
C	1.234000	-2.210000	-3.914000
H	2.110000	-1.576000	-3.973000
C	0.953000	0.479000	-5.195000
H	1.852000	0.049000	-5.624000
C	-0.013000	-4.668000	-1.421000
C	-1.034000	4.833000	-1.485000
H	-1.947000	5.206000	-1.038000
C	1.104000	-5.119000	-0.695000
H	2.017000	-5.381000	-1.219000
C	0.097000	-4.022000	-2.756000
C	-0.123000	-0.357000	-4.847000
C	0.039000	-1.799000	-4.525000
C	-1.119000	4.237000	-2.736000
H	-2.088000	4.184000	-3.219000
C	-0.012000	3.587000	-3.311000
C	-1.018000	-3.777000	-3.578000
H	-1.910000	-4.385000	-3.471000
C	1.230000	3.839000	-2.703000
H	2.133000	3.418000	-3.128000
C	-1.316000	1.633000	-4.120000
H	-2.199000	2.036000	-3.640000
C	-1.302000	0.281000	-4.430000
H	-2.172000	-0.313000	-4.179000

[8]CPP:

80

00000001

C	-5.496000	1.645000	1.844000
H	-5.639000	1.982000	2.864000
C	-5.323000	0.274000	1.582000
C	-4.845000	-0.682000	2.613000
C	-3.919000	-0.220000	3.561000
H	-3.777000	0.846000	3.694000
C	-3.040000	-1.086000	4.192000
H	-2.252000	-0.655000	4.794000
C	-3.042000	-2.464000	3.917000
C	-1.801000	-3.252000	4.144000
C	-0.749000	-2.761000	4.937000
H	-0.937000	-1.987000	5.670000
C	0.565000	-3.146000	4.711000
H	1.348000	-2.625000	5.250000
C	0.898000	-4.068000	3.703000
C	-2.244000	4.048000	-3.070000
C	-2.382000	4.444000	-1.728000
H	-1.591000	5.001000	-1.243000
C	-3.424000	3.984000	-0.940000
H	-3.401000	4.197000	0.122000

C	-4.386000	3.097000	-1.446000
C	-5.088000	2.203000	-0.490000
C	-5.159000	0.831000	-0.780000
H	-4.963000	0.487000	-1.788000
C	-5.274000	-0.112000	0.233000
H	-5.164000	-1.160000	-0.019000
C	-4.998000	-2.075000	2.511000
H	-5.763000	-2.486000	1.861000
C	-4.122000	-2.944000	3.153000
H	-4.238000	-4.009000	2.987000
C	-3.339000	3.361000	-3.629000
H	-3.342000	3.114000	-4.684000
C	-4.380000	2.891000	-2.837000
H	-5.158000	2.290000	-3.295000
C	-1.491000	-4.352000	3.326000
H	-2.268000	-4.826000	2.738000
C	-0.180000	-4.760000	3.125000
H	0.003000	-5.561000	2.420000
C	-5.382000	2.588000	0.830000
H	-5.439000	3.641000	1.082000
C	5.496000	-1.645000	-1.844000
H	5.639000	-1.982000	-2.864000
C	5.323000	-0.274000	-1.582000
C	4.845000	0.682000	-2.613000
C	3.919000	0.220000	-3.561000
H	3.777000	-0.846000	-3.694000
C	3.040000	1.086000	-4.192000
H	2.252000	0.655000	-4.794000
C	3.042000	2.464000	-3.917000
C	1.801000	3.252000	-4.144000
C	0.749000	2.761000	-4.937000
H	0.937000	1.987000	-5.670000
C	-0.565000	3.146000	-4.711000
H	-1.348000	2.625000	-5.250000
C	-0.898000	4.068000	-3.703000
C	2.244000	-4.048000	3.070000
C	2.382000	-4.444000	1.728000
H	1.591000	-5.001000	1.243000
C	3.424000	-3.984000	0.940000
H	3.401000	-4.197000	-0.122000
C	4.386000	-3.097000	1.446000
C	5.088000	-2.203000	0.490000
C	5.159000	-0.831000	0.780000
H	4.963000	-0.487000	1.788000
C	5.274000	0.112000	-0.233000
H	5.164000	1.160000	0.019000
C	4.998000	2.075000	-2.511000
H	5.763000	2.486000	-1.861000
C	4.122000	2.944000	-3.153000
H	4.238000	4.009000	-2.987000
C	3.339000	-3.361000	3.629000
H	3.342000	-3.114000	4.684000
C	4.380000	-2.891000	2.837000
H	5.158000	-2.290000	3.295000
C	1.491000	4.352000	-3.326000

H	2.268000	4.826000	-2.738000
C	0.180000	4.760000	-3.125000
H	-0.003000	5.561000	-2.420000
C	5.382000	-2.588000	-0.830000
H	5.439000	-3.641000	-1.082000

[9]CPP:

90

00000001

C	0.676000	-6.174000	0.069000
C	1.509000	-6.136000	-1.062000
H	1.109000	-6.388000	-2.037000
C	2.812000	-5.667000	-0.983000
H	3.362000	-5.535000	-1.907000
C	3.369000	-5.239000	0.234000
C	2.619000	-5.523000	1.389000
H	3.025000	-5.307000	2.369000
C	1.304000	-5.961000	1.308000
H	0.728000	-6.027000	2.223000
C	4.511000	-4.286000	0.256000
C	4.675000	-3.414000	1.346000
H	4.126000	-3.584000	2.263000
C	5.394000	-2.234000	1.230000
H	5.377000	-1.531000	2.055000
C	5.981000	-1.856000	0.014000
C	5.994000	-2.819000	-1.009000
H	6.509000	-2.605000	-1.939000
C	5.286000	-4.008000	-0.885000
H	5.280000	-4.693000	-1.725000
C	6.249000	-0.416000	-0.221000
C	5.729000	0.175000	-1.382000
H	5.369000	-0.456000	-2.186000
C	5.492000	1.540000	-1.449000
H	4.953000	1.921000	-2.307000
C	5.774000	2.389000	-0.366000
C	6.498000	1.823000	0.701000
H	6.829000	2.448000	1.521000
C	6.720000	0.453000	0.777000
H	7.207000	0.045000	1.656000
C	5.067000	3.691000	-0.254000
C	4.439000	4.294000	-1.358000
H	4.715000	4.003000	-2.364000
C	3.372000	5.168000	-1.192000
H	2.827000	5.492000	-2.071000
C	2.898000	5.509000	0.085000
C	3.693000	5.110000	1.173000
H	3.431000	5.426000	2.176000
C	4.739000	4.214000	1.009000
H	5.229000	3.832000	1.896000
C	1.500000	5.969000	0.273000
C	0.754000	6.634000	-0.717000
H	1.264000	7.096000	-1.555000
C	0.784000	5.486000	1.380000
H	1.307000	4.967000	2.172000

C	-0.804000	-6.128000	-0.046000
C	-1.381000	-5.588000	-1.207000
H	-0.768000	-5.409000	-2.081000
C	-2.683000	-5.112000	-1.216000
H	-3.036000	-4.584000	-2.093000
C	-3.479000	-5.143000	-0.061000
C	-2.971000	-5.853000	1.040000
H	-3.581000	-5.976000	1.928000
C	-1.668000	-6.339000	1.044000
H	-1.300000	-6.834000	1.935000
C	-4.623000	-4.201000	0.027000
C	-4.782000	-3.425000	1.185000
H	-4.237000	-3.688000	2.083000
C	-5.473000	-2.220000	1.152000
H	-5.446000	-1.580000	2.027000
C	-6.035000	-1.737000	-0.039000
C	-6.061000	-2.618000	-1.135000
H	-6.567000	-2.322000	-2.048000
C	-5.372000	-3.823000	-1.102000
H	-5.354000	-4.446000	-1.989000
C	-6.262000	-0.277000	-0.186000
C	-5.772000	0.356000	-1.338000
H	-5.459000	-0.245000	-2.184000
C	-5.506000	1.716000	-1.355000
H	-4.994000	2.123000	-2.218000
C	-5.724000	2.521000	-0.226000
C	-6.412000	1.923000	0.846000
H	-6.691000	2.517000	1.709000
C	-6.667000	0.556000	0.870000
H	-7.129000	0.121000	1.749000
C	-4.987000	3.806000	-0.095000
C	-4.407000	4.445000	-1.205000
H	-4.743000	4.203000	-2.206000
C	-3.316000	5.292000	-1.061000
H	-2.814000	5.643000	-1.955000
C	-2.769000	5.570000	0.202000
C	-3.514000	5.140000	1.313000
H	-3.196000	5.409000	2.314000
C	-4.584000	4.269000	1.169000
H	-5.034000	3.858000	2.064000
C	-1.353000	5.999000	0.334000
C	-0.637000	6.649000	-0.686000
H	-1.171000	7.124000	-1.501000
C	-0.600000	5.500000	1.409000
H	-1.099000	4.991000	2.224000

[10]CPP:

100

00000001

C	-6.840000	-2.970000	-0.847000
H	-7.037000	-3.631000	-1.682000
C	-6.841000	2.970000	0.847000
H	-7.038000	3.631000	1.682000
C	-7.279000	-1.653000	-0.923000
H	-7.794000	-1.318000	-1.817000

C	-7.000000	-0.735000	0.102000
C	-4.559000	5.156000	-1.295000
H	-4.907000	4.897000	-2.288000
C	-5.971000	2.554000	-1.342000
H	-5.410000	2.855000	-2.217000
C	-7.279000	1.653000	0.923000
H	-7.794000	1.318000	1.817000
C	-7.000000	0.735000	-0.102000
C	-6.081000	3.426000	-0.246000
C	-5.971000	-2.555000	1.341000
H	-5.410000	-2.855000	2.217000
C	-6.081000	-3.427000	0.246000
C	-6.426000	1.245000	-1.275000
H	-6.206000	0.573000	-2.096000
C	-5.201000	-4.622000	0.165000
C	-5.201000	4.622000	-0.165000
C	-6.426000	-1.246000	1.275000
H	-6.206000	-0.573000	2.096000
C	-4.762000	5.095000	1.084000
H	-5.247000	4.758000	1.991000
C	-3.628000	-5.885000	-1.201000
H	-3.292000	-6.171000	-2.191000
C	-3.408000	5.924000	-1.178000
H	-2.875000	6.200000	-2.080000
C	-4.559000	-5.156000	1.295000
H	-4.907000	-4.897000	2.288000
C	-4.761000	-5.095000	-1.084000
H	-5.247000	-4.758000	-1.991000
C	-3.408000	-5.924000	1.178000
H	-2.874000	-6.200000	2.080000
C	-2.855000	6.223000	0.078000
C	-3.628000	5.885000	1.201000
H	-3.293000	6.170000	2.191000
C	-1.427000	-6.605000	-0.208000
C	-0.696000	-7.260000	0.798000
H	-1.219000	-7.739000	1.618000
C	-1.427000	6.605000	0.208000
C	-2.855000	-6.223000	-0.078000
C	-0.692000	-6.086000	-1.286000
H	-1.206000	-5.564000	-2.083000
C	0.696000	-7.260000	0.798000
H	1.220000	-7.739000	1.618000
C	-0.692000	6.086000	1.286000
H	-1.206000	5.564000	2.083000
C	6.840000	2.970000	0.847000
H	7.037000	3.631000	1.682000
C	6.841000	-2.970000	-0.847000
H	7.038000	-3.631000	-1.682000
C	7.279000	1.653000	0.923000
H	7.794000	1.318000	1.817000
C	7.000000	0.735000	-0.102000
C	4.559000	-5.156000	1.295000
H	4.907000	-4.897000	2.288000
C	5.971000	-2.554000	1.342000
H	5.410000	-2.855000	2.217000

C	7.279000	-1.653000	-0.923000
H	7.794000	-1.318000	-1.817000
C	7.000000	-0.735000	0.102000
C	6.081000	-3.426000	0.246000
C	5.971000	2.555000	-1.341000
H	5.410000	2.855000	-2.217000
C	6.081000	3.427000	-0.246000
C	6.426000	-1.245000	1.275000
H	6.206000	-0.573000	2.096000
C	5.201000	4.622000	-0.165000
C	5.201000	-4.622000	0.165000
C	6.426000	1.246000	-1.275000
H	6.206000	0.573000	-2.096000
C	4.762000	-5.095000	-1.084000
H	5.248000	-4.758000	-1.991000
C	3.628000	5.885000	1.201000
H	3.292000	6.171000	2.191000
C	3.408000	-5.924000	1.178000
H	2.875000	-6.200000	2.080000
C	4.559000	5.156000	-1.295000
H	4.907000	4.897000	-2.288000
C	4.761000	5.095000	1.084000
H	5.247000	4.758000	1.991000
C	3.408000	5.924000	-1.178000
H	2.874000	6.200000	-2.080000
C	2.855000	-6.223000	-0.078000
C	3.628000	-5.885000	-1.201000
H	3.293000	-6.170000	-2.191000
C	1.427000	6.605000	0.208000
C	0.696000	7.260000	-0.798000
H	1.219000	7.739000	-1.618000
C	1.427000	-6.605000	-0.208000
C	2.855000	6.223000	0.078000
C	0.692000	6.086000	1.286000
H	1.206000	5.564000	2.083000
C	-0.696000	7.260000	-0.798000
H	-1.220000	7.739000	-1.618000
C	0.692000	-6.086000	-1.286000
H	1.206000	-5.564000	-2.083000

[11]CPP:

110

00000001

C	4.963000	5.778000	-0.152000
C	6.010000	4.725000	-0.110000
C	6.665000	4.266000	-1.264000
H	6.627000	4.857000	-2.173000
C	4.087000	5.816000	-1.247000
H	4.303000	5.218000	-2.124000
C	2.871000	6.481000	-1.172000
H	2.169000	6.389000	-1.993000
C	2.473000	7.132000	0.004000
C	1.038000	7.457000	0.187000
C	0.232000	7.982000	-0.834000

H	0.696000	8.400000	-1.721000
C	-1.154000	7.907000	-0.763000
H	-1.733000	8.283000	-1.599000
C	-1.803000	7.300000	0.327000
C	-3.216000	6.839000	0.266000
C	-3.865000	6.296000	1.388000
H	-3.440000	6.420000	2.376000
C	-4.997000	5.505000	1.259000
H	-5.386000	5.005000	2.138000
C	-5.562000	5.238000	0.003000
C	-6.451000	4.064000	-0.175000
C	-7.320000	3.598000	0.826000
H	-7.560000	4.238000	1.668000
C	-7.834000	2.306000	0.791000
H	-8.464000	1.969000	1.607000
C	-7.508000	1.419000	-0.249000
C	-7.685000	-0.050000	-0.150000
C	-7.738000	-0.874000	-1.285000
H	-7.928000	-0.435000	-2.258000
C	3.420000	7.239000	1.036000
H	3.175000	7.800000	1.931000
C	6.177000	3.974000	1.063000
H	5.691000	4.295000	1.976000
C	4.639000	6.574000	0.959000
H	5.326000	6.631000	1.796000
C	0.390000	7.027000	1.353000
H	0.978000	6.635000	2.175000
C	-0.993000	6.951000	1.421000
H	-1.432000	6.501000	2.301000
C	-5.038000	5.948000	-1.088000
H	-5.487000	5.834000	-2.069000
C	-3.894000	6.726000	-0.960000
H	-3.474000	7.167000	-1.856000
C	-6.246000	3.224000	-1.281000
H	-5.575000	3.538000	-2.071000
C	-6.763000	1.939000	-1.318000
H	-6.479000	1.290000	-2.138000
C	-7.474000	-2.233000	-1.205000
H	-7.449000	-2.798000	-2.128000
C	-7.141000	-2.852000	0.014000
C	-7.282000	-2.058000	1.166000
H	-7.101000	-2.480000	2.146000
C	-7.541000	-0.697000	1.087000
H	-7.519000	-0.111000	1.999000
C	7.592000	0.747000	-0.229000
C	7.320000	2.204000	-0.151000
C	7.306000	3.032000	-1.285000
H	7.753000	2.683000	-2.208000
C	7.075000	0.022000	-1.313000
H	6.644000	0.555000	-2.153000
C	6.959000	-1.359000	-1.264000
H	6.441000	-1.872000	-2.066000
C	7.366000	-2.084000	-0.133000
C	6.838000	-3.459000	0.056000
C	6.691000	-4.369000	-1.001000

H	7.215000	-4.194000	-1.935000
C	5.829000	-5.454000	-0.905000
H	5.717000	-6.094000	-1.771000
C	5.065000	-5.692000	0.252000
C	3.855000	-6.560000	0.242000
C	3.056000	-6.719000	1.387000
H	3.431000	-6.427000	2.359000
C	1.743000	-7.160000	1.307000
H	1.140000	-7.153000	2.208000
C	1.151000	-7.481000	0.076000
C	-0.326000	-7.532000	-0.049000
C	-1.170000	-7.859000	1.027000
H	-0.757000	-8.335000	1.909000
C	-2.521000	-7.536000	1.009000
H	-3.128000	-7.767000	1.877000
C	-3.098000	-6.871000	-0.087000
C	-4.402000	-6.172000	-0.010000
C	-5.157000	-5.859000	-1.152000
H	-4.934000	-6.346000	-2.095000
C	8.022000	-1.374000	0.884000
H	8.404000	-1.908000	1.748000
C	6.818000	2.742000	1.043000
H	6.817000	2.136000	1.942000
C	8.134000	0.012000	0.837000
H	8.604000	0.534000	1.664000
C	6.198000	-3.781000	1.261000
H	6.285000	-3.109000	2.107000
C	5.342000	-4.868000	1.357000
H	4.803000	-5.001000	2.285000
C	2.002000	-7.499000	-1.041000
H	1.617000	-7.812000	-2.005000
C	3.312000	-7.048000	-0.960000
H	3.888000	-7.000000	-1.876000
C	-0.939000	-7.015000	-1.200000
H	-0.332000	-6.745000	-2.056000
C	-2.289000	-6.697000	-1.220000
H	-2.689000	-6.190000	-2.090000
C	-6.143000	-4.883000	-1.121000
H	-6.646000	-4.642000	-2.049000
C	-6.436000	-4.163000	0.052000
C	-5.811000	-4.619000	1.226000
H	-6.018000	-4.143000	2.175000
C	-4.824000	-5.594000	1.196000
H	-4.293000	-5.819000	2.114000

[12]CPP:

120

00000001

C	-6.625000	5.008000	0.156000
C	-6.461000	5.928000	-0.894000
H	-7.116000	5.883000	-1.756000
C	-5.442000	6.872000	-0.872000
H	-5.331000	7.540000	-1.718000
C	-4.520000	6.927000	0.189000

C	-4.797000	6.124000	1.306000
H	-4.129000	6.137000	2.158000
C	-5.833000	5.201000	1.297000
H	-5.935000	4.529000	2.140000
C	-3.209000	7.613000	0.077000
C	-2.603000	7.789000	-1.178000
H	-3.172000	7.607000	-2.082000
C	-1.252000	8.081000	-1.295000
H	-0.819000	8.160000	-2.286000
C	-0.426000	8.176000	-0.163000
C	-1.066000	8.175000	1.087000
H	-0.479000	8.286000	1.991000
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H	-2.865000	7.879000	2.192000
C	1.048000	8.055000	-0.268000
C	1.936000	8.504000	0.724000
H	1.577000	9.154000	1.514000
C	3.264000	8.089000	0.747000
H	3.905000	8.428000	1.553000
C	3.773000	7.217000	-0.230000
C	2.924000	6.899000	-1.301000
H	3.269000	6.228000	-2.078000
C	1.598000	7.298000	-1.314000
H	0.955000	6.924000	-2.101000
C	5.059000	6.491000	-0.095000
C	5.557000	6.132000	1.167000
H	5.108000	6.548000	2.061000
C	6.526000	5.146000	1.305000
H	6.831000	4.859000	2.304000
C	7.045000	4.467000	0.190000
C	6.696000	4.978000	-1.072000
H	7.104000	4.530000	-1.969000
C	5.729000	5.963000	-1.211000
H	5.446000	6.280000	-2.208000
C	7.753000	3.169000	0.310000
C	7.587000	2.376000	1.456000
H	7.074000	2.776000	2.321000
C	7.920000	1.030000	1.462000
H	7.652000	0.448000	2.334000
C	8.455000	0.395000	0.329000
C	8.794000	1.235000	-0.748000
H	9.291000	0.827000	-1.619000
C	8.455000	2.581000	-0.756000
H	8.702000	3.169000	-1.632000
C	8.403000	-1.085000	0.202000
C	8.379000	-1.701000	-1.062000
H	8.626000	-1.130000	-1.948000
C	7.933000	-3.006000	-1.228000
H	7.877000	-3.418000	-2.229000
C	7.466000	-3.758000	-0.140000
C	7.656000	-3.209000	1.138000
H	7.342000	-3.768000	2.012000
C	8.119000	-1.911000	1.303000
H	8.190000	-1.518000	2.309000
C	6.609000	-4.954000	-0.320000

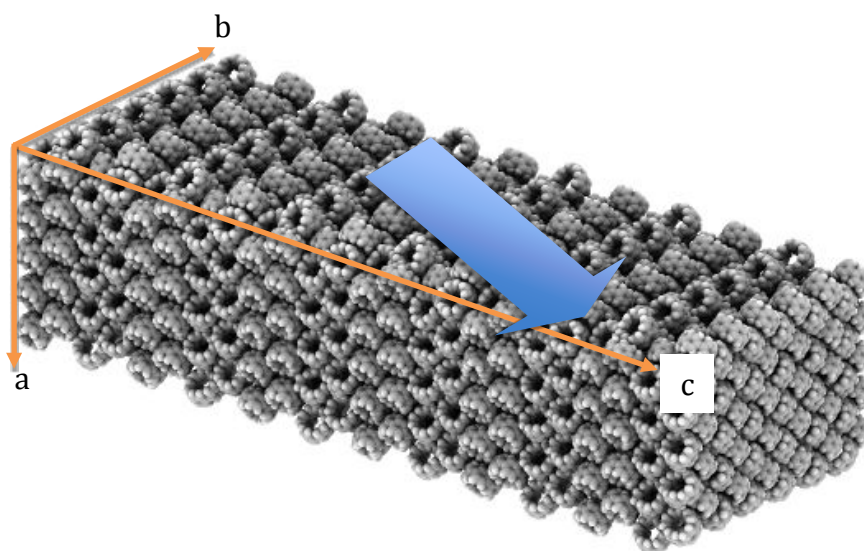
C	6.548000	-6.010000	0.603000
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H	5.472000	-7.710000	1.327000
C	4.483000	-6.845000	-0.386000
C	4.636000	-5.883000	-1.396000
H	3.870000	-5.776000	-2.155000
C	5.670000	-4.960000	-1.362000
H	5.683000	-4.163000	-2.096000
C	3.187000	-7.555000	-0.259000
C	2.642000	-7.814000	1.009000
H	3.254000	-7.679000	1.894000
C	1.296000	-8.113000	1.167000
H	0.904000	-8.245000	2.169000
C	0.426000	-8.162000	0.066000
C	1.011000	-8.093000	-1.209000
H	0.386000	-8.166000	-2.091000
C	2.359000	-7.799000	-1.367000
H	2.757000	-7.690000	-2.369000
C	-1.044000	-8.067000	0.230000
C	-1.965000	-8.506000	-0.736000
H	-1.629000	-9.134000	-1.553000
C	-3.301000	-8.120000	-0.690000
H	-3.970000	-8.458000	-1.474000
C	-3.781000	-7.267000	0.318000
C	-2.888000	-6.944000	1.351000
H	-3.204000	-6.283000	2.148000
C	-1.561000	-7.339000	1.313000
H	-0.891000	-6.972000	2.080000
C	-5.077000	-6.548000	0.233000
C	-5.647000	-6.217000	-1.007000
H	-5.252000	-6.658000	-1.915000
C	-6.631000	-5.244000	-1.116000
H	-6.997000	-4.992000	-2.104000
C	-7.075000	-4.522000	0.005000
C	-6.631000	-4.981000	1.257000
H	-6.971000	-4.496000	2.164000
C	-5.672000	-5.976000	1.369000
H	-5.331000	-6.259000	2.357000
C	-7.777000	-3.219000	-0.118000
C	-7.734000	-2.487000	-1.316000
H	-7.360000	-2.950000	-2.220000
C	-8.042000	-1.136000	-1.358000
H	-7.907000	-0.620000	-2.299000
C	-8.371000	-0.420000	-0.194000
C	-8.602000	-1.193000	0.958000
H	-8.952000	-0.725000	1.869000
C	-8.325000	-2.552000	0.992000
H	-8.481000	-3.084000	1.922000
C	-8.302000	1.064000	-0.157000
C	-8.383000	1.778000	1.053000
H	-8.698000	1.279000	1.961000
C	-7.950000	3.093000	1.150000
H	-7.964000	3.578000	2.119000
C	-7.440000	3.777000	0.035000

C	-7.580000	3.143000	-1.209000
H	-7.245000	3.645000	-2.109000
C	-7.990000	1.821000	-1.300000
H	-7.991000	1.359000	-2.278000

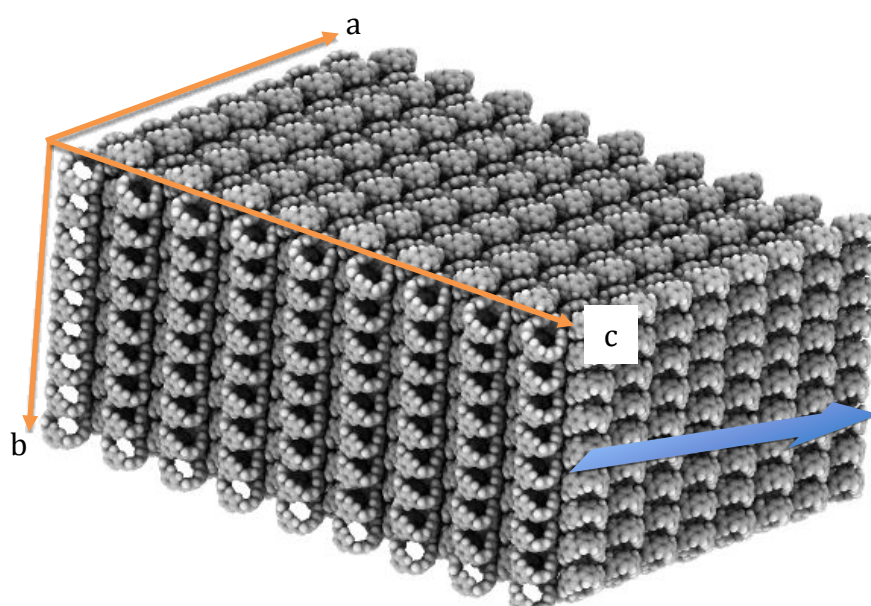
S2. Representative MD snapshots of [n]CPPs equilibrated at 300K

Blue arrows show the charge transport direction with the maximum mobility.

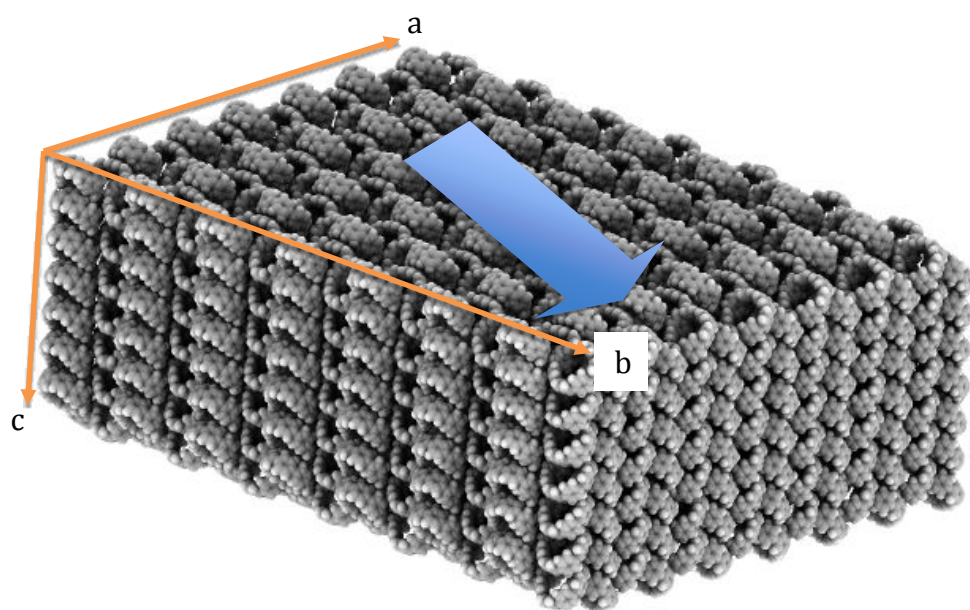
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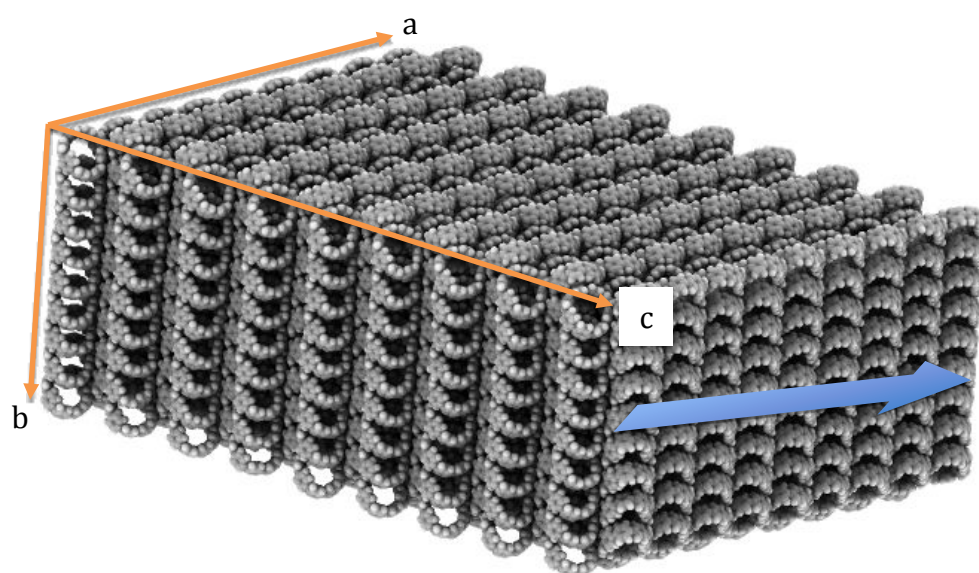
[6]CPP:



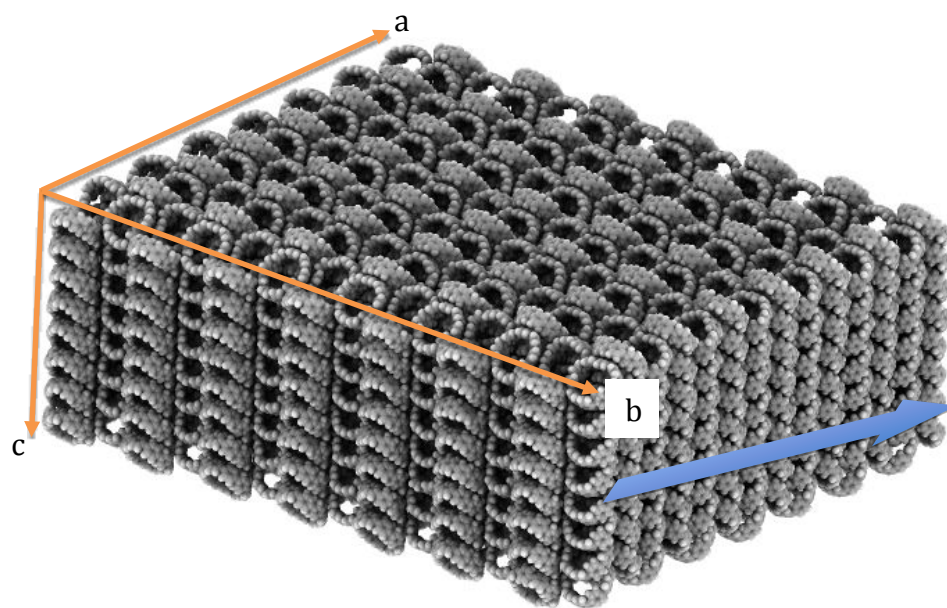
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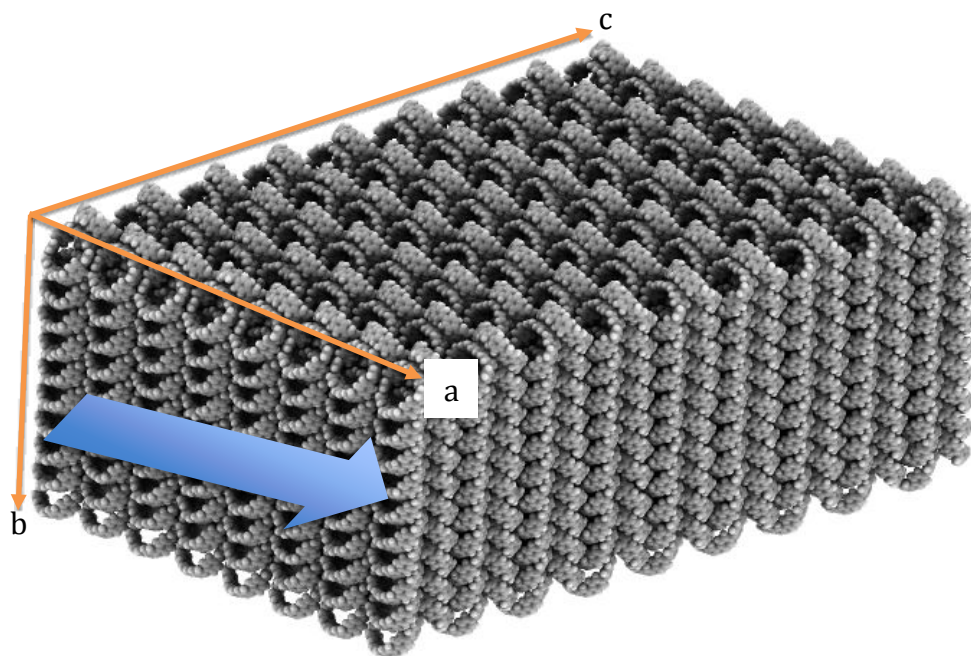
[8]CPP:



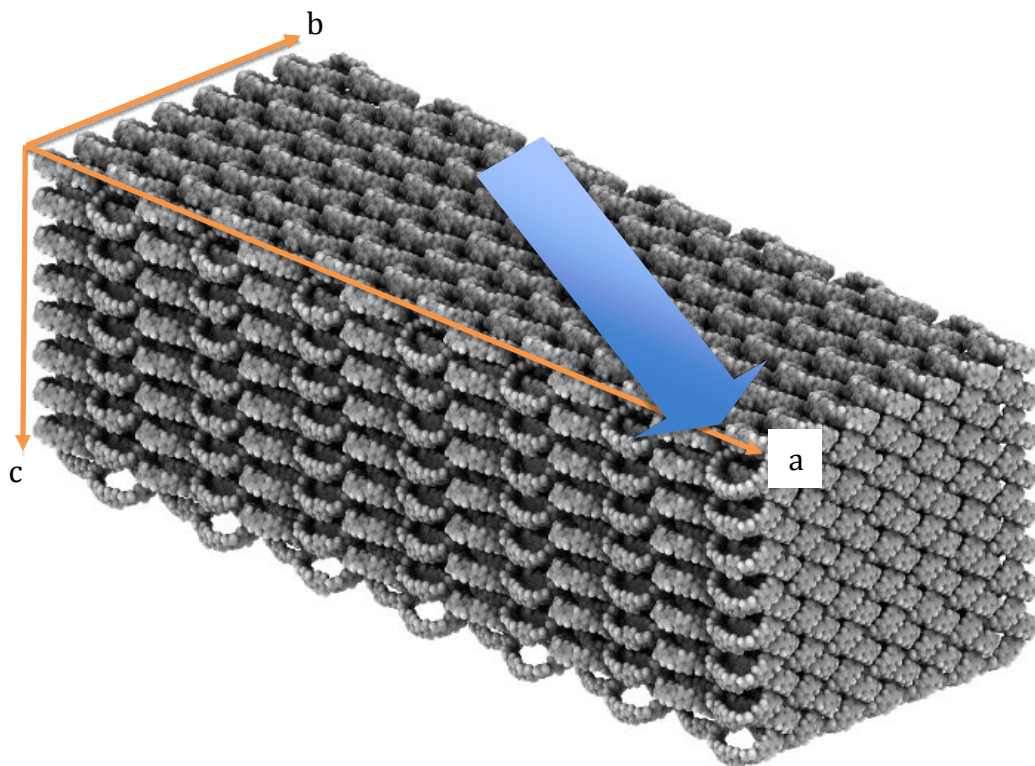
[9]CPP:



[10]CPP:



[11]CPP:



[12]CPP:

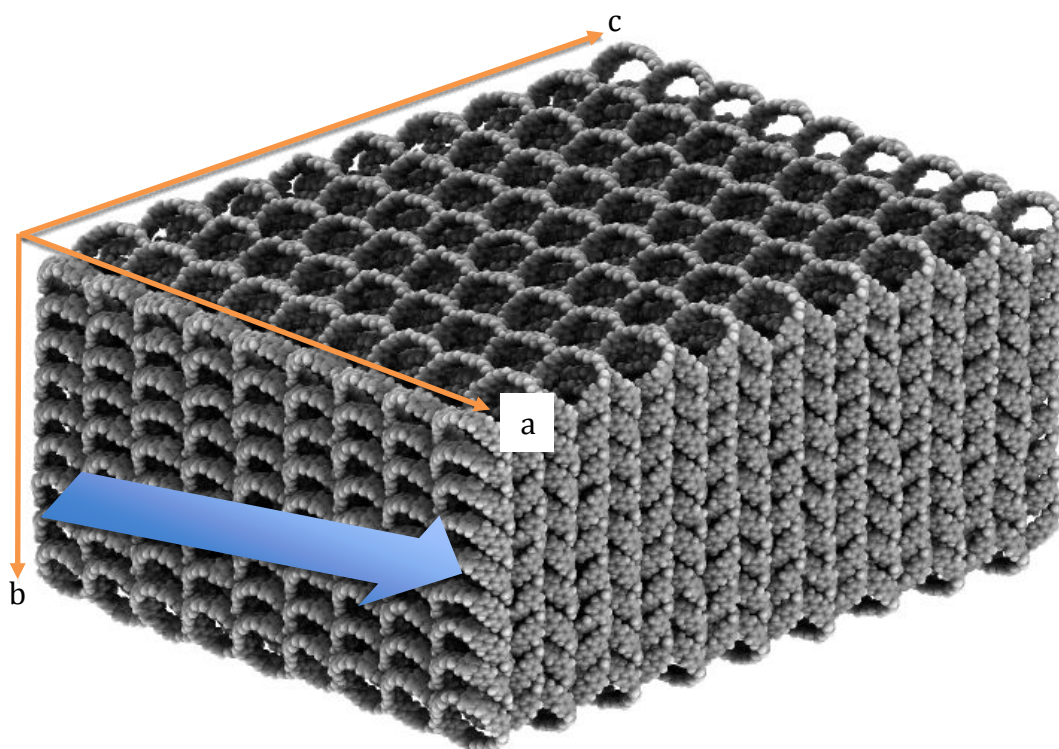


Table S1. Experimental unit-cell parameters vs. predicted unit-cell parameters extracted from MD equilibrated supercells at 300K.

[n]CPP	Experimental (XRD)						
	a	b	c		α (°)	β (°)	γ (°)
5	9.8322	11.6273	35.5547		90.00	90.00	90.00
6	11.1580	8.1773	15.8360		90.00	105.32	90.00
7	18.3400	22.3350	8.2180		90.00	90.00	90.00
8	12.9325	8.0103	19.3676		90.00	105.36	90.00
9	20.9873	26.5941	8.0799		90.00	90.00	90.00
10	15.9075	8.1405	20.7418		90.00	108.66	90.00
11	36.8303	13.7639	10.2794		90.00	90.00	90.00
12	18.5827	8.1878	23.6701		90.00	106.16	90.00

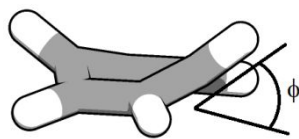
[n]CPP	Predicted by MD (AMBER/GAFF)			% difference
	a	b	c	
5	9.9592	11.7775	36.01383	1.28
6	11.285	8.270111	16.01633	1.13
7	18.5477	22.5877	8.3110	1.12
8	13.1152	8.1236	19.6413	1.12
9	21.5689	27.3310	8.3038	2.70
10	16.1709	8.2753	21.0852	1.63
11	37.1401	13.8797	10.3659	0.83
12	18.9077	8.3310	24.0841	1.72

Table S2. MD equilibrated supercell parameters

[n]CPP	k*a (Å)	l*b (Å)	m*c (Å)	# of molecules
5	49.796	70.665	216.083	1440
6	90.280	74.431	144.147	1296
7	129.834	158.114	58.177	1372
8	118.037	73.112	176.772	1458
9	150.982	191.317	66.430	1568
10	129.367	82.753	189.767	1440
11	259.981	97.158	82.927	1568
12	170.169	74.979	216.757	1458

Here k, l and m are integers and represent that unit-cells are repeated k, l and m times along the crystallographic directions a, b and c, respectively.

Table S3. Strain per phenyl ring found from B3LYP/6-311G(d,p)



[n]CPP	$\phi(^{\circ})$
5	13.6
6	11.7
7	10.0
8	8.8
9	7.9
10	7.1
11	6.6
12	5.3