# Supplementary info

***SI.4. data related to Flory-Higgins interaction parameter for all cellulose variants.***

# Interaction parameters calculated from molecular dynamics

Table S. 1. At STP condition calculated values of *Xij,* mixing energy (*Emix*) and energy of formed complex (*Ebs*) at 298 K

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ***i*** | ***j*** | ***Xij,*** | ***Emix*** (kcal/mol) | ***Eij avg*** (kcal/mol) |
| CH2OH | CH2OH | 0 | 0 | -1.90994641 |
|  | H2O | -1.25775834 | -0.74482881 | -2.20353938 |
|  | COONa | 7.93710466 | 4.70025446 | -0.85380554 |
|  | COOH | -8.47843226 | -5.02082192 | -2.53338385 |
|  | COO | 6.79519086 | 4.02402734 | -0.5488944 |
|  | CHO | 5.01320897 | 2.96875987 | -0.55496748 |
|  | CNF ring | -1.58867227 | -0.94079192 | -2.53407729 |
| H2O | CH2OH | -1.25775834 | -0.74482881 | -2.20353938 |
|  | H2O | 0 | 0 | -2.30778495 |
|  | COONa | 11.12301353 | 6.58690998 | -0.68175479 |
|  | COOH | -14.43749519 | -8.54970471 | -3.30281245 |
|  | COO | 9.77825227 | 5.79055913 | -0.4178535 |
|  | CHO | 6.11254968 | 3.61977574 | -0.62706699 |
|  | CNF ring | -9.79980432 | -5.80332198 | -3.30686462 |
| COONa | CH2OH | 7.93710466 | 4.70025446 | -0.85380554 |
|  | H2O | 11.12301353 | 6.58690998 | -0.68175479 |
|  | COONa | 0 | 0 | -1.50379335 |
|  | COOH | 4.90900649 | 2.90705246 | -0.89386312 |
|  | COO | 1.04452272 | 0.61855334 | -0.96053391 |
|  | CHO | 3.0868092 | 1.82796994 | -0.55581363 |
|  | CNF ring | 2.56198663 | 1.51717655 | -1.97957794 |
| COOH | CH2OH | -8.47843226 | -5.02082192 | -2.53338385 |
|  | H2O | -14.43749519 | -8.54970471 | -3.30281245 |
|  | COONa | 4.90900649 | 2.90705246 | -0.89386312 |
|  | COOH | 0 | 0 | -1.34303702 |
|  | COO | 3.9472867 | 2.33753399 | -0.57096975 |
|  | CHO | 1.97779403 | 1.17122498 | -0.59623068 |
|  | CNF ring | 1.73641587 | 1.02828384 | -1.93341719 |
| COO | CH2OH | 6.79519086 | 4.02402734 | -0.5488944 |
|  | H2O | 9.77825227 | 5.79055913 | -0.4178535 |
|  | COONa | 1.04452272 | 0.61855334 | -0.96053391 |
|  | COOH | 3.9472867 | 2.33753399 | -0.57096975 |
|  | COO | 0 | 0 | -0.64508442 |
|  | CHO | 0.77570342 | 0.4593619 | -0.37699264 |
|  | CNF ring | 5.67684352 | 3.36175598 | -1.19851858 |
| CHO | CH2OH | 5.01320897 | 2.96875987 | -0.55496748 |
|  | H2O | 6.11254968 | 3.61977574 | -0.62706699 |
|  | COONa | 3.0868092 | 1.82796994 | -0.55581363 |
|  | COOH | 1.97779403 | 1.17122498 | -0.59623068 |
|  | COO | 0.77570342 | 0.4593619 | -0.37699264 |
|  | CHO | 0 | 0 | -0.27510059 |
|  | CNF ring | 7.27009437 | 4.30525928 | -0.85013758 |
| CNF ring | CH2OH | -1.58867227 | -0.94079192 | -2.53407729 |
|  | H2O | -9.79980432 | -5.80332198 | -3.30686462 |
|  | COONa | 2.56198663 | 1.51717655 | -1.97957794 |
|  | COOH | 1.73641587 | 1.02828384 | -1.93341719 |
|  | COO | 5.67684352 | 3.36175598 | -1.19851858 |
|  | CHO | 7.27009437 | 4.30525928 | -0.85013758 |
|  | CNF ring | 0 | 0 | -3.07381354 |
| CNF = cellulose nanofibril | | | | |