**Supplementary information**

***SI.3. COSMO charge densities for all cellulose variants.***

COSMO sigma charge densities

DFT calculations for all cellulose variants. The variants include:

|  |  |
| --- | --- |
| **ID** | **Description of cellulose variant** |
| B | cellulose molecules with CH2OH functional groups (native cellulose) |
| D | cellulose molecules with –CHO functional groups |
| F | cellulose molecules with –COOH functional groups |
| G | cellulose molecules with –COONa functional groups |
| H | cellulose molecules with –COONa functional groups (dissociated Na) |
| W | cellulose molecules with –COO‒ functional groups |

Our Herein, the cellulose model consists of 16 glucose residues. Therefore, there’s 16 CH2OH functional groups on native cellulose model that can be replaced by the groups listed. Thus, 16 of each variant can be realized (ordered replacement of functional group from one side (leftmost) to the other side(rightmost)). This replacement is referred as degree of substation (DOS).

The atomic coordination of DFT relaxed structures are provided in “S6.xyz.rar” file. Following naming convention is used for the files archived in “xyz.tar”: ***DOS***.***ID***. where ***DOS*** is a number showing how many CH2OH functional groups are replaced by the associated functional groups in variant ***ID***.

|  |  |
| --- | --- |
| File ID | COSMO sigma charge density |
| 00.B |  |
| 01.D |  |
| 01.F |  |
| 01.G |  |
| 01.H |  |
| 01.W |  |
| 02.D |  |
| 02.F |  |
| 02.G |  |
| 02.H |  |
| 02.W |  |
| 03.D | A picture containing table, man, different, people  Description automatically generated |
| 03.F | A close up of a map  Description automatically generated |
| 03.G | A group of people around each other  Description automatically generated |
| 03.H | A screenshot of a cell phone  Description automatically generated |
| 03.W | A group of people on a map  Description automatically generated |
| 04.D | A picture containing map, water, different, kite  Description automatically generated |
| 04.F | A picture containing man, different, table, water  Description automatically generated |
| 04.G | A picture containing map, water, different, group  Description automatically generated |
| 04.H |  |
| 04.W | A picture containing man, water, table, group  Description automatically generated |
| 05.D | A group of people on a map  Description automatically generated |
| 05.F | A picture containing map, man, different, water  Description automatically generated |
| 05.G | A picture containing different, table, man, group  Description automatically generated |
| 05.H | A map of a person  Description automatically generated |
| 05.W | A close up of a map  Description automatically generated |
| 06.D | A map of a person  Description automatically generated |
| 06.F | A group of people on a map  Description automatically generated |
| 06.G | A group of people on a beach  Description automatically generated |
| 06.H | A close up of a map  Description automatically generated |
| 06.W | A group of people on a map  Description automatically generated |
| 07.D | A picture containing man, table, different, group  Description automatically generated |
| 07.F | A group of people in different colors  Description automatically generated |
| 07.G | A picture containing man, different, table, water  Description automatically generated |
| 07.H | A picture containing outdoor, map, man, water  Description automatically generated |
| 07.W | A group of people around each other  Description automatically generated |
| 08.D | A close up of a person  Description automatically generated |
| 08.F | A group of people in different colors  Description automatically generated |
| 08.H | A close up of a map  Description automatically generated |
| 08.W | A group of people around each other  Description automatically generated |
| 09.D | A picture containing man, different, water, table  Description automatically generated |
| 09.F | A group of people in different colors  Description automatically generated |
| 09.G | A picture containing water, different, table, man  Description automatically generated |
| 09.H | A close up of a map  Description automatically generated |
| 09.W | A picture containing man, water, kite, different  Description automatically generated |
| 10.D | A screenshot of a cell phone  Description automatically generated |
| 10.F | A picture containing man, different, water, table  Description automatically generated |
| 10.G | A picture containing map, water, group, table  Description automatically generated |
| 10.H | A close up of a map  Description automatically generated |
| 10.W | A picture containing man, different, table, water  Description automatically generated |
| 11.D | A picture containing different, man, table, group  Description automatically generated |
| 11.F | A picture containing man, table, group, people  Description automatically generated |
| 11.G | A picture containing man, different, table, water  Description automatically generated |
| 11.H | A picture containing map, water, man  Description automatically generated |
| 11.W | A picture containing man, group  Description automatically generated |
| 12.D | A picture containing table, man, different, water  Description automatically generated |
| 12.F | A group of people on a map  Description automatically generated |
| 13.G | A group of people on a map  Description automatically generated |
| 13.H | A close up of a map  Description automatically generated |
| 13.W | A close up of a person  Description automatically generated |
| 14.D | A close up of a person  Description automatically generated |
| 14.F | A close up of a person  Description automatically generated |
| 14.G | A close up of a map  Description automatically generated |
| 14.H | A picture containing map, man, table  Description automatically generated |
| 14.W | A picture containing map, man  Description automatically generated |
| 15.D | A close up of a person  Description automatically generated |
| 15.F | A close up of a person  Description automatically generated |
| 15.G | A screenshot of a map  Description automatically generated |
| 15.H | A picture containing white, man  Description automatically generated |
| 15.W | A close up of a person  Description automatically generated |
| 16.D | A screenshot of a cell phone  Description automatically generated |
| 16.F | A picture containing man, table, different, people  Description automatically generated |
| 16.G |  |
| 16.H | A picture containing water, man, table, light  Description automatically generated |
| 16.W | A picture containing table, man  Description automatically generated |