Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Multiscale modelling investigation of wood modification with acetic anhydride

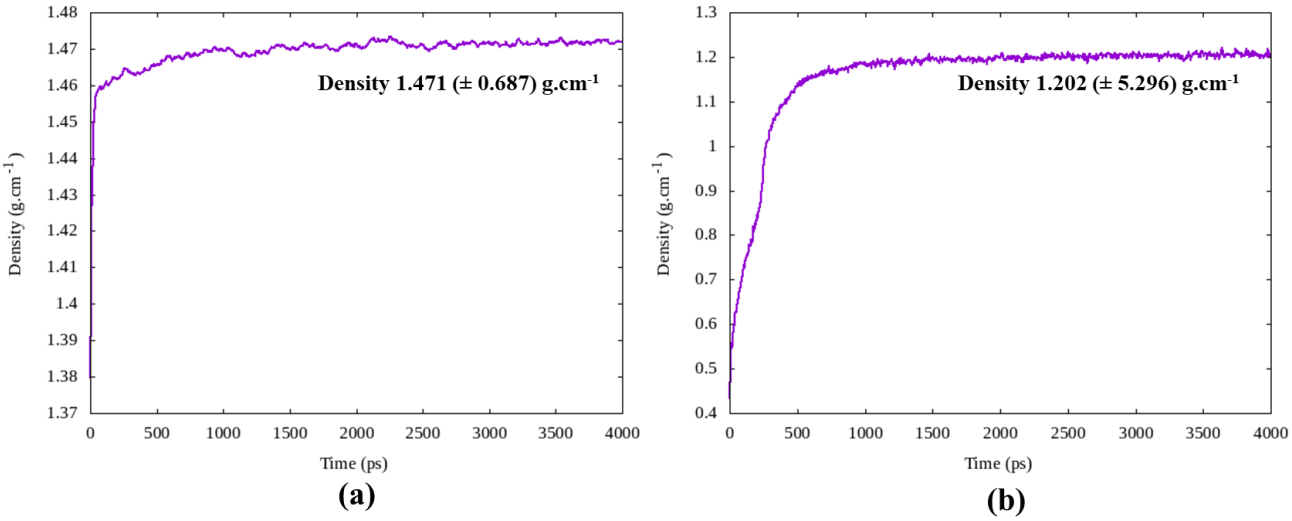

Fig. S1 Simulated density of (a) pure cellobiose at 300 K and (b) pure lignin-model at 298.15 K. The density values were computed with final 2 ns.

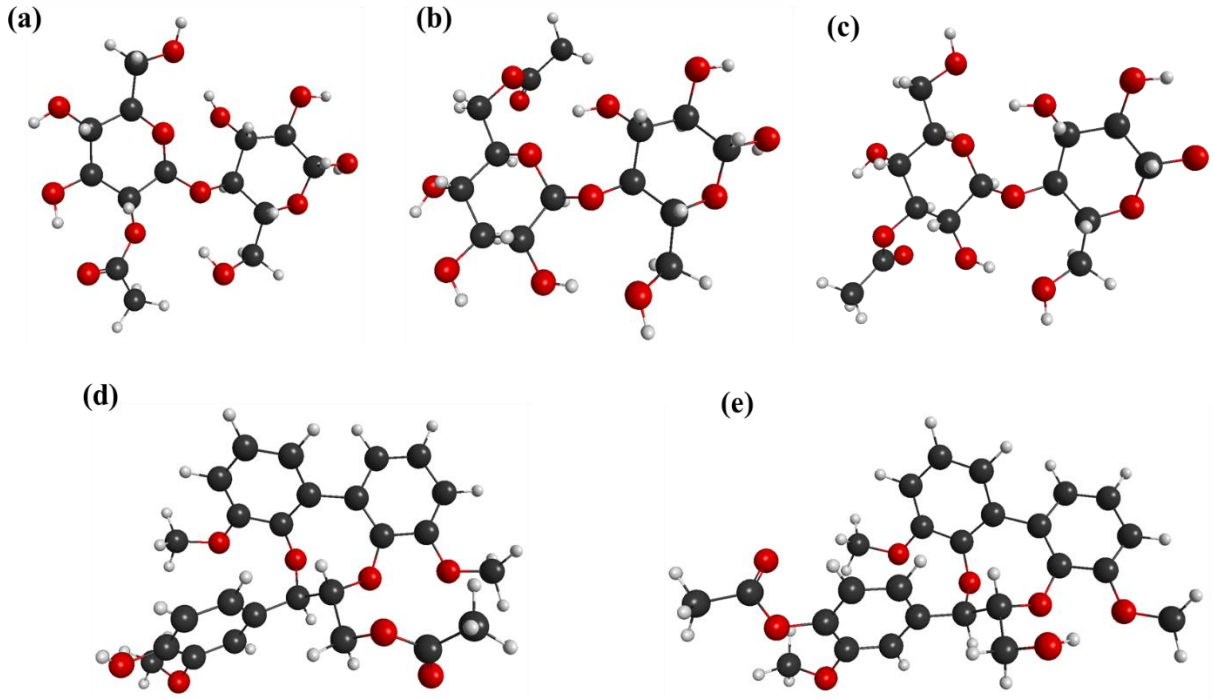

Fig. S2 Optimized structures of acetylated cellobiose and acetylated lignin model in gas phase: (a) acetylated cellobiose at HO-(C2) position, (b) acetylated cellobiose at HO-(C6) position, (c) acetylated cellobiose at HO-(C3) position, (d) acetylated lignin at HO-(γ)-aliphatic position, and (e) acetylated lignin at HO-(C4)-aromatic position.

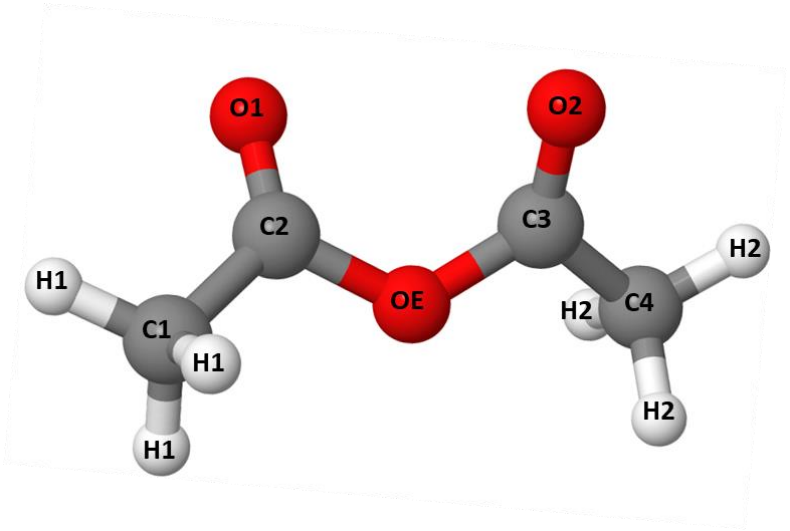

Fig. S3 Atom labelling of acetic anhydride molecule.