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Investigating Fundamental Interactions between Pectin and Cellulose Nanocrystals: A Molecular Dynamics Simulation

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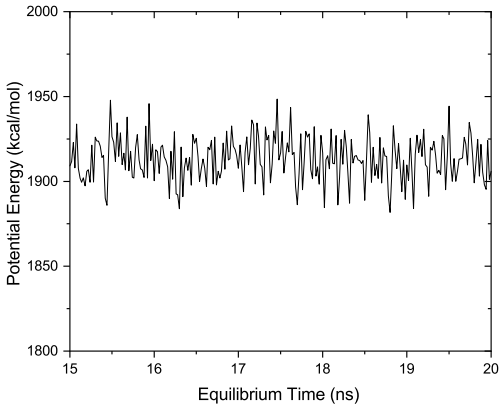
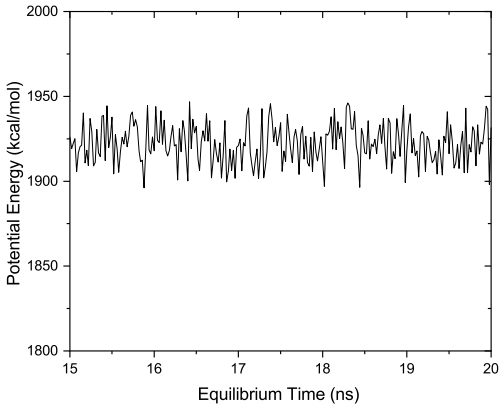
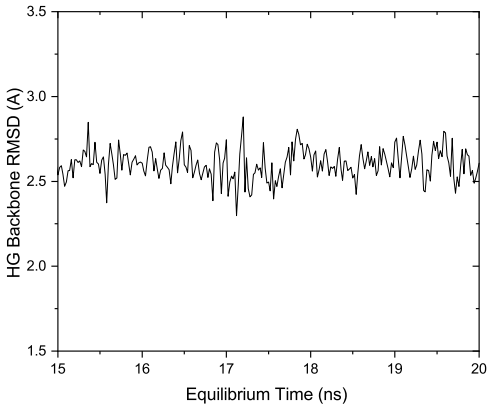


(a)

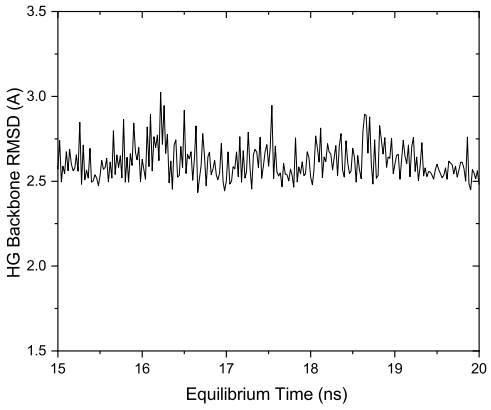


(b)

Fig. S1 The potential energies of (a) an HG-50 and (b) an HG-0 molecule during the last 5 ns of equilibrium.

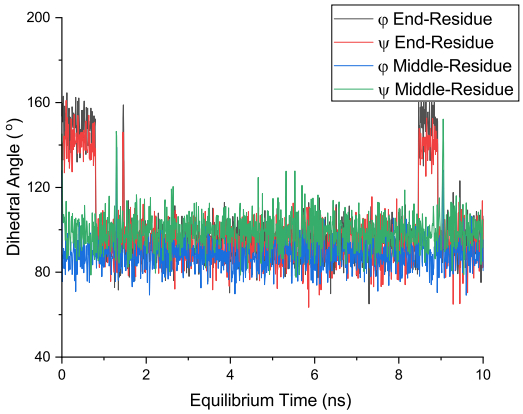


(a)

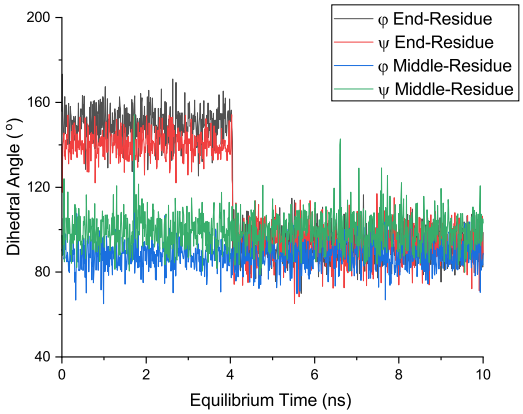


(b)

Fig. S2 The RMSD of backbone atoms of (a) an HG-50 and (b) an HG-0 molecule during the last 5 ns equilibrium.

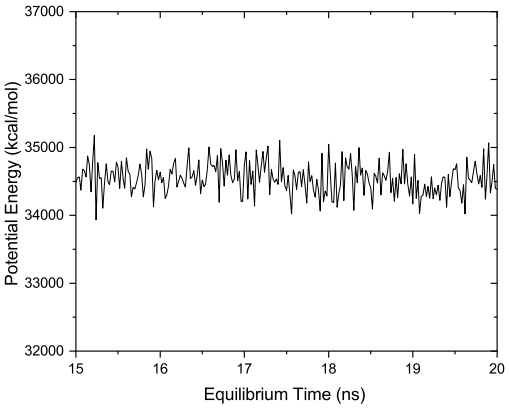


(a)

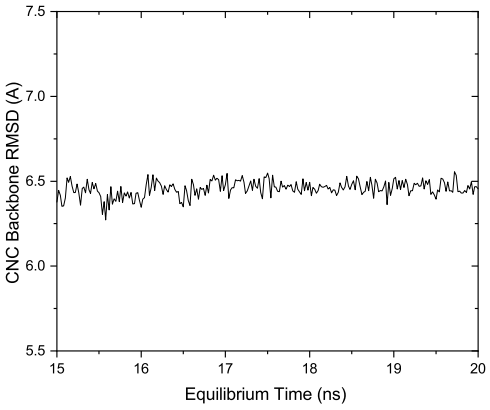


(b)

Fig. S3 The dihedral angles of (a) an HG-50 and (b) an HG-0 molecule during a 10 ns equilibrium.



(a)



(b)

Fig. S4 The last 5 ns equilibrium of a CNC particle at 300K and (a) the potential energy and (b) the RMSD of backbone atoms are shown for equilibrium state.

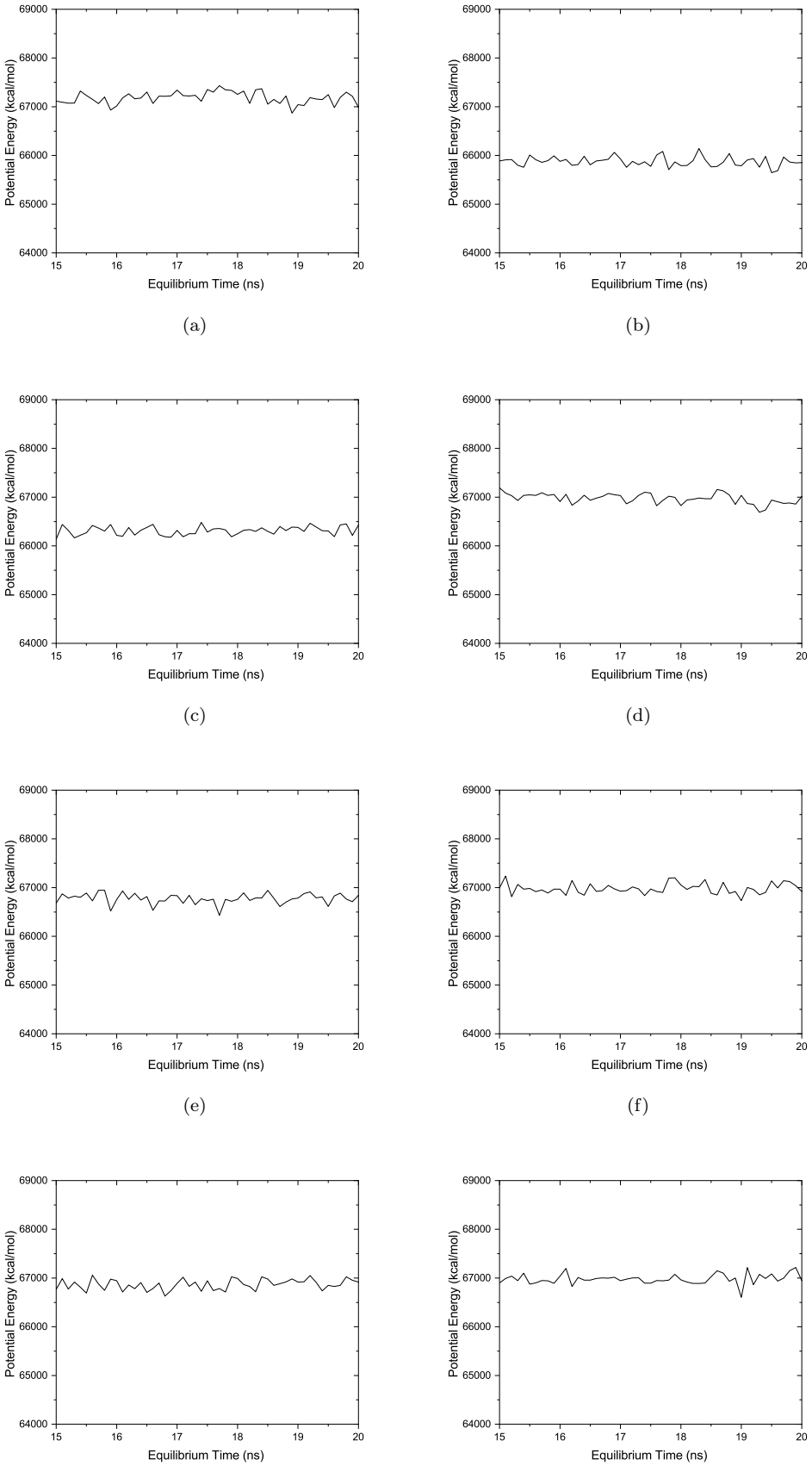


Fig. S5 The last 5 ns of potential energies in the equilibrium simulation of the baseline models (a) (200)/(200), (b) (110)/(110) and the interphase models with (c,d) HG-100, (e,f) HG-50 and (g,h) HG-0 molecules between the CNC (200) and (110) surfaces, in the left and right columns, respectively.

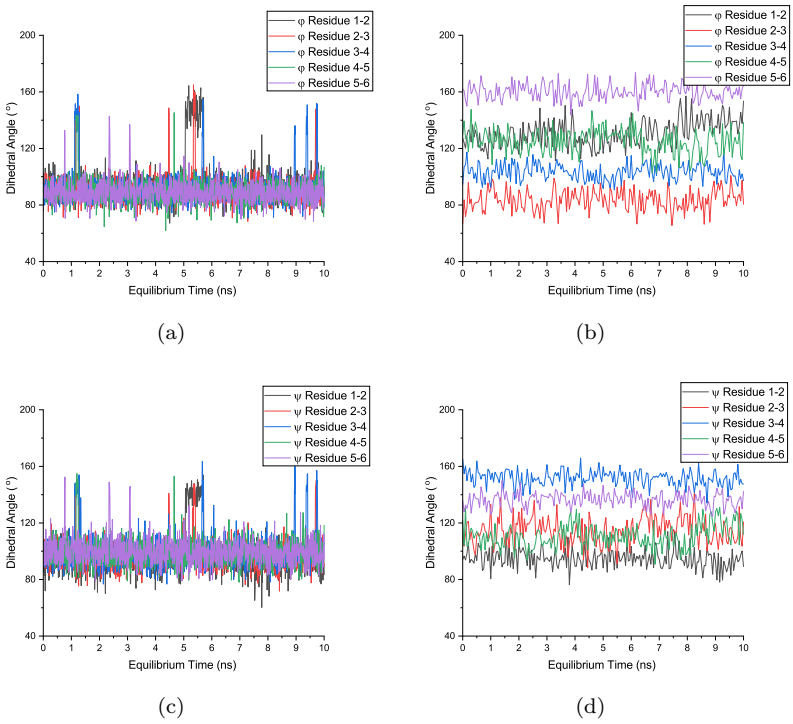


Fig. S6 (a,c) The dihedral angles in a HG-100 molecule equilibrium in a vacuum. The angles are constant inside a molecule. (b,d) After being physically absorbed between CNC (200) surfaces, the dihedral angles vary through a pectin molecule, reflecting local HG/CNC interaction.