DFT computational studies of cellulose molecules adsorption on carbon nanostructures

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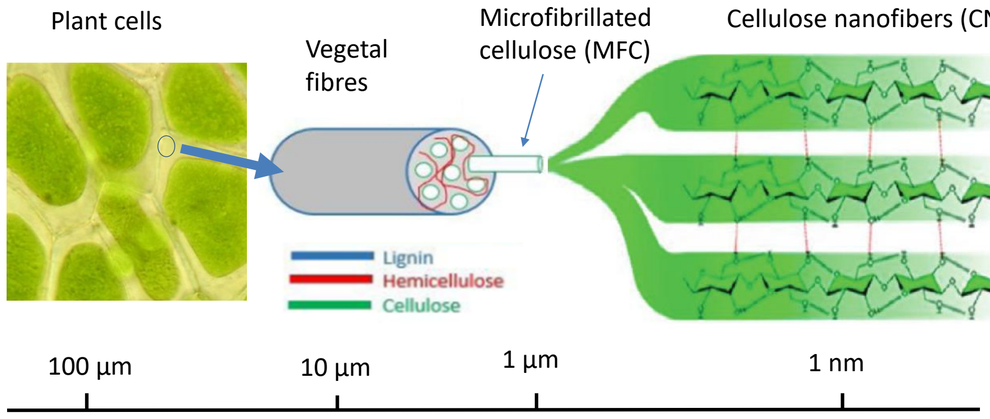
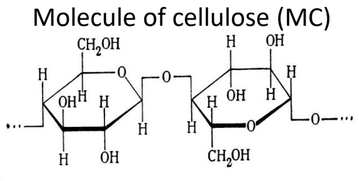
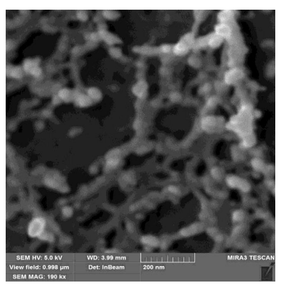
Introduction and calculation methods





Structure of nanocellulose

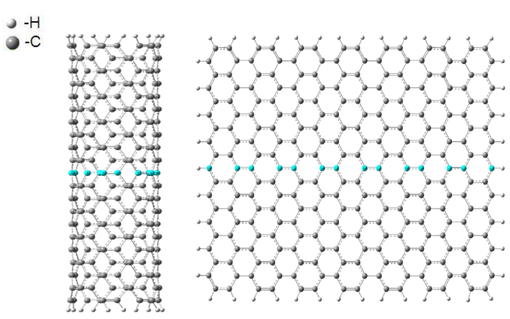


The needs of modern electronics require elaboration of hybrid composite materials with unique properties. The composite materials, where the matrix is micro/nanosized cellulose and carbon nanostructure is a filler, reveal some advantages that allowed their practical use in many applications.

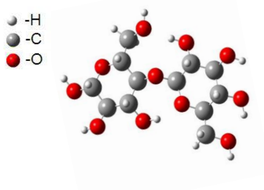
The ab-initio electronic structure calculations can provide important information about interactions between the components of the composites and ensure successful elaboration of materials with optimized characteristics. The work presents results of the computational studies of cellulose molecules adsorption on the surfaces of carbon nanostructures –sheets and fragments of nanotubes. Both molecules and adsorbents were considered as molecular clusters (fragments). The DFT - based geometry-optimized calculations of electronic structures of carbon nanostructures with adsorbed molecules were carried out by Gaussian 09 program package.

Results

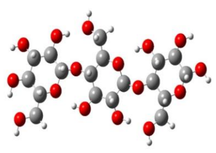
Component of investigated structures:



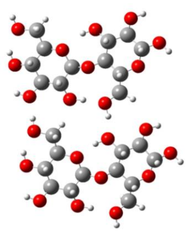
Carbon nanotube (CNT) (5,5) and graphene.



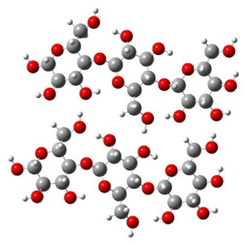
Cluster MC(2)



Cluster MC(3)

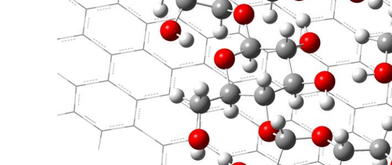
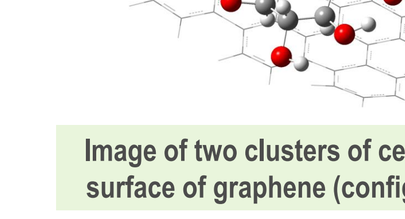


Cluster MC(2+2)



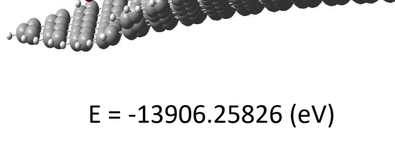
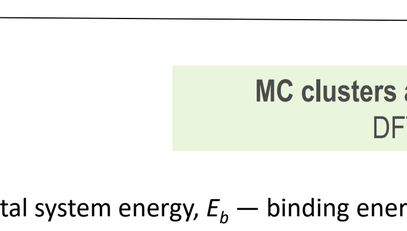
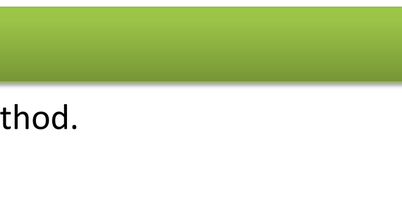
Cluster MC(3+3)

Adsorbed structures:

Configuration of system	R^{min}, Å (type of bound)
①  E = -9310.644229 (eV) E_b = -0.002808 (eV)	3.05 (H-C)
②  E = -9921.193982 (eV) E_b = -0.003415 (eV)	3.07 (H-C) 3.19 (H-C) 3.22 (H-C) 3.24 (H-C)

MC clusters adsorbed on CNT (5,5).
DFT b3lyp/6-31G

Image of two clusters of cellulose on the surface of graphene (configuration №6).

Configuration of system	R^{min}, Å (type of bound)
③  E = -11400.56064 (eV)	2.32 (H-C) 2.52 (H-C)
④  E = -12007.95478 (eV)	2.41 (H-C) 2.41 (H-C) 2.45 (H-C) 2.48 (H-C)
⑤  E = -12691.41013 (eV)	2.37 (H-C) 2.27 (H-C) 2.62 (H-C)
⑥ E = -13906.25826 (eV)	2.27 (O-H) 2.4 (H-C) 2.24 (H-C) 2.46 (H-C) 2.37 (H-C)

MC clusters adsorbed on graphene.
DFT b3lyp/3-21G

E — total system energy, E_b — binding energy, R^{min} — smallest distance between atoms.

Conclusions

- Geometric configurations of cellulose atoms and carbon structures were obtained by the DFT method.
- MC (2) and MC (3) are not adsorbed on CNTs, as evidenced by low values of binding energy E_b .
- It was found that adsorption on the surface of graphene is quite possible, as the smallest distances between atoms R^{min} = 2.3 Å – 2.4 Å for MC and graphene are smaller compared to R^{min} for MC and CNTs (3 Å – 3.1 Å).