Molecular modeling of small molecules thin film on the surface

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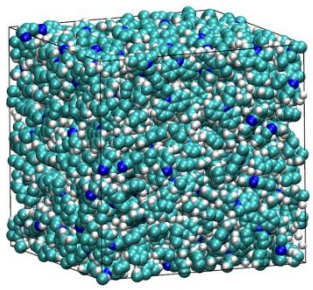
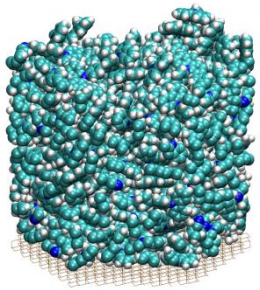
The electronic properties of amorphous organic thin films are of great interest, because they can be used in organic light-emitting diodes (OLED) displays and other devices. Compared to conventional inorganic semiconductors, amorphous organic thin films have the potential to cover larger areas and create some devices on flexible substrates.

In this study, two methods of modeling amorphous organic thin films, consisted of 4-4'-N,N'-Dicarbazolylbiphenyl (CBP) molecules, have been implemented. The first method is based on the molecular dynamics compression of the unit cell with molecules located randomly inside it with low initial density. As a result, we obtained an amorphous isotropic material structure. Then it becomes possible to further simulate generated material by molecular dynamics. The second algorithm imitates the process of vacuum deposition. The main goal of such method is getting anisotropic packing near a flat surface, because the detailed investigation of molecular orientation and ordering in such materials is very important for explaining the relationship between the chemical characteristics of single molecules and physical properties of the films. All molecular dynamics calculations were performed with the aid of GROMACS [1] package.





The molecular orientation of OLED materials in vacuum-deposited amorphous films has been investigated. Also the time dependence of the molecular orientation and mean square displacement of the molecules were calculated at different temperatures. These data can serve as a measure of the molecular mobility in the material.

The results indicate that CBP molecules perfectly oriented horizontally to the substrate surface at the room temperature. Also these molecules have low diffusion rate. It means that for determining of values of different physical parameters we have to average over several cells generated independently, not only over one trajectory.

Recently experiments show that the horizonlal orientation of the transition dipole moment of emitting molecules positively affects on charge transport and light outcoupling [2], because the light is emitting mainly in the direction orthogonal to the transition dipole moment.

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[1] D. van der Spoel, E. Lindahl, B. Hess, A.R. van Buuren, E. Apol, P.J. Meulenhoff, D.P. Tieleman, A.L.T.M. Sijbers, K.A. Feenstra, R. van Drunen, and H.J.C. Berendsen, *Gromacs user manual version 4.5*, www.gromacs.org, **2010**

[2] D. Yokoyama, *J. Mater. Chem.*, **2011**, *V. 21*, P. 19187