Modeling of the structure and properties of amorphous layers for organic light-emitting diodes

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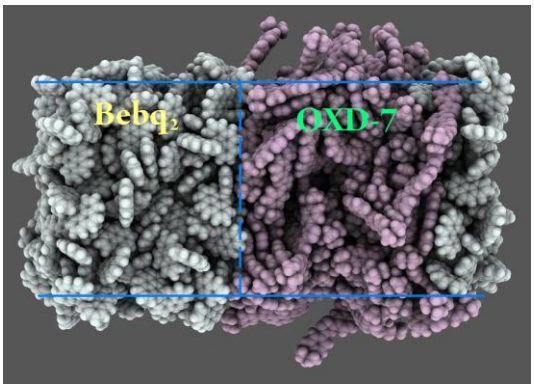
The geometrical structure and electronic properties of an 1,3-bis[2-(4-tert-butylphenyl)-1,3,4-oxadiazol-5-yl]benzene (OXD-7) electron-transporting layer, an emitting layer composed of beryllium complexes ($Bebq_2$, $Be[4\text{-}mpp]_2$, $Bepp_2$), and an interface between these two layers are studied by MD simulations combined with quantum-chemical DFT/TDDFT calculations for sample structures along MD trajectories. The AMBER force field has been used in MD simulations. Because some important force-field parameters are lacking in the AMBER force field, these parameters have been estimated by fitting AMBER potential energy scans to results of first-principles calculations.



The estimated force constants have been verified by available experimental data (densities and crystal structure). Amorphous layers composed of OXD-7, $Bebq_2$, $Be[4\text{-}mpp]_2$ and Bepp2 molecules and the interfaces between the OXD-7 layer and the $Bebq_2$, $Be[4\text{-}mpp]_2$ and Bepp2 layers have been built using the GROMACS software package. HOMO and LUMO energy level distributions and the band shape of the absorption spectra of molecules in the amorphous layers have been calculated by the DFT and TDDFT methods. The layer structures and calculated distributions can then be used for charge-transfer modeling.