A theoretical analysis of the role of exciplexes in light emission in OLEDs: the structure and spectroscopic properties of α-NPD−BAlq exciplexes at an α-NPD/BAlq interface

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Abstract Light emission in layered OLEDs is often attributed to exciplexes formed at the interface between two neighboring layers of organic materials [1, 2]. In this work, the structure and spectroscopic properties of exciplexes formed at an interface between a layer of hole-transporting N,N'-di(naphthalen-2-yl)-N,N'-diphenyl-benzidine (α-NPD) and a layer of electron transporting bis(2-methyl-8-quinolinato)(4-phenylphenolato)aluminum (BAlq) have been investigated theoretically by multiscale (molecular dynamics, MD, and quantum chemistry, QC) simulations. Such an interface is typical for organic light-emitting devices. The GROMACS and ORCA packages have been used for MD and QC calculations, respectively. The two adjacent disordered layers have been constructed by simulating sequential gas-phase deposition of α-NPD and BAlq onto a solid 3Å-thick tetragonal substrate formed by two layers of sp3-hybridized carbon atoms (as at a graphene surface). The thickness of both the α-NPD and BAlq layers is 10 nm; these layers contain 230 α-NPD and 250 BAlq molecules, respectively. Then, a central 5-nm slab has been cut from the constructed 20-nm bilayer at the interface (Fig. 1). Four α-NPD−BAlq pairs have been selected in this slab for the subsequent QC investigation. The geometrical parameters of these pairs (molecular complexes) have been fully optimized at the DFT PBE0/SV(P) level. The binding energies (BE) have been calculated as differences between the total energy of the geometrically optimized complex and the total energies of isolated molecules. The calculated BE are in the range from –17.4 to –21.5 kcal/mol. The energies of the first ten excited states in the studied complexes have been calculated using time-dependent density functional theory (TDDFT) with different exchange-correlation functionals taking into account different amounts of Hartree–Fock exchange (PBE0 and BHHLYP). The geometries of complexes in the first excited state have been calculated using the TDDFT/BHHLYP approximation with inclusion of the D3BJ dispersion corrections. The binding energies in the exciplexes have been were calculated as differences between the total energies of the complexes optimized in the first excited state (CT state) and the total energies of α-NPD in the ground state and BAlq in the first excited state. The calculated binding energies of the exciplexes are in the range from 21.9 to 34.1 kcal/mol.

References

[1] Zhu Wen-qing, Jiang Xue-yin, Zhang Zhi-lin, J. Shanghai University (English Edition), **10 no. 2** (2006) 156–160.
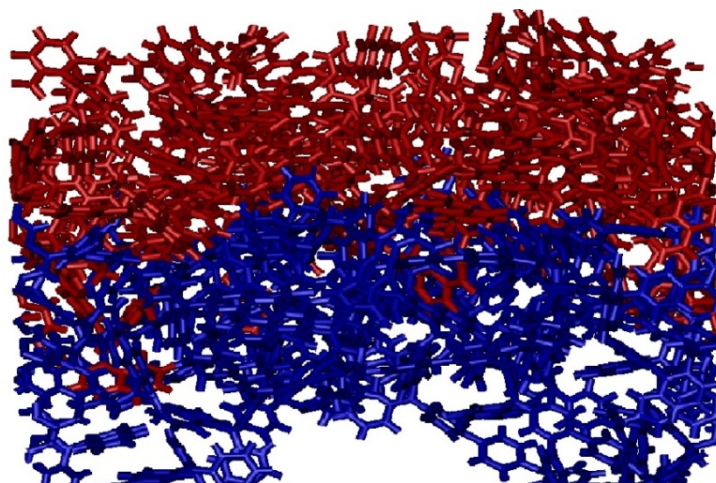[2] M. Carvelli, A. van Reenen, R.A.J. Janssen, H.P. Loebl, R. Coehoorn, Organic Electronics **13** (2012) 2605–2614.

Figures

Fig. 1. Central layer with the interface.