Research Digest
Apr. 1, 2012

Molecular orientation in OLEDs

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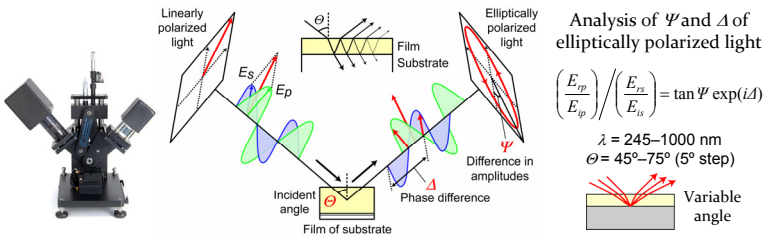
Review paper

D. Yokoyama, "Molecular orientation in small-molecule organic light-emitting diodes"
***J. Mater. Chem.* 21, 19187 (2011) [Feature Article]**

1. Characterization

Variable angle spectroscopic ellipsometry (VASE)



Analysis of Ψ and Δ of elliptically polarized light

$$\left(\frac{E_{rp}}{E_{ip}}\right)\Big/\left(\frac{E_{rs}}{E_{is}}\right) = \tan\Psi\exp(i\Delta)$$

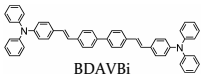
λ = 245–1000 nm
Θ = 45°–75° (5° step)

Optical property of film

***n*: Refractive index**
***k*: Extinction coefficient**

Electronic property of molecule

Molecular polarizability
Transition dipole moment



Ordinary (horizontal) n_o, k_o — Extraordinary (vertical) n_e, k_e

Optical anisotropy

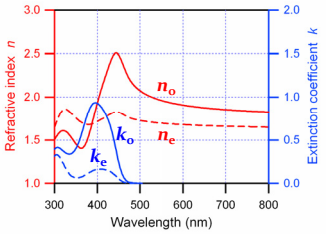
Electronic anisotropy

Molecular polarizability (Å³)

$$\begin{pmatrix} 291 & -20 & 0 \\ -20 & 80 & 0 \\ 0 & 0 & 57 \end{pmatrix}$$

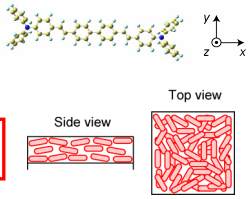
Transition dipole moment (Debye)

$$\begin{pmatrix} 15.8 \\ -1.3 \\ 0 \end{pmatrix}$$

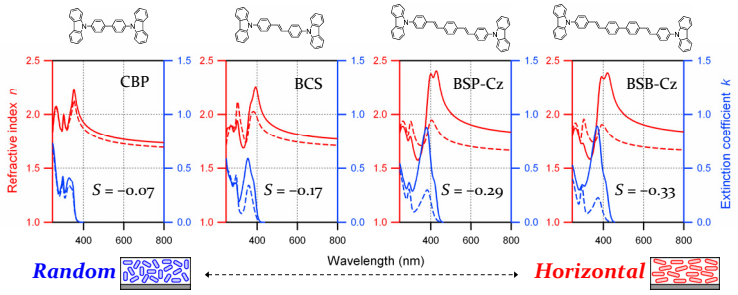


$n_o > n_e$
$k_o > k_e$

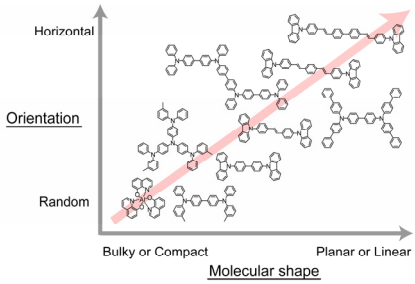
Horizontal orientation

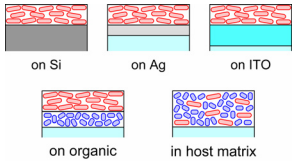


Dependence on molecular length



General properties



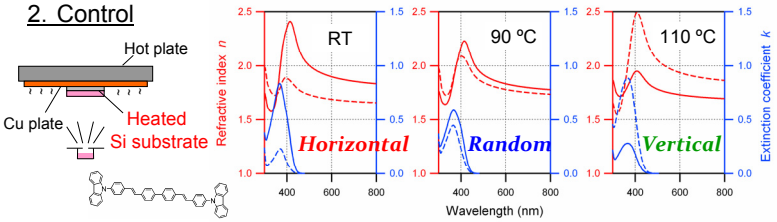


The larger the anisotropy of molecular shape is, the more significant the horizontal orientation is.

The horizontal orientation occurs on any underlying layers and even in a doped film.

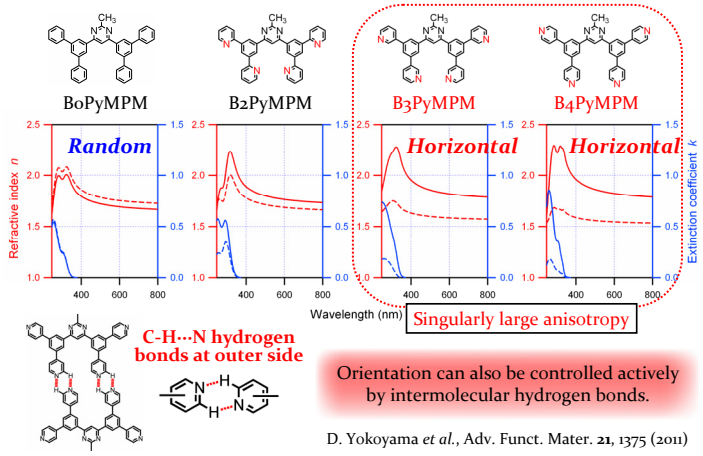
D. Yokoyama *et al.*, *Org. Electron.* **10**, 127 (2009); *Appl. Phys. Lett.* **93**, 173302 (2008)

2. Control



Orientation can be controlled by deposition on a heated substrate even at a temperature lower than T_g.

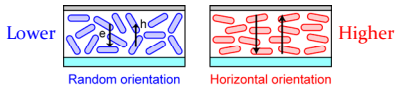
D. Yokoyama *et al.*, *J. Appl. Phys.* **107**, 123512 (2010)



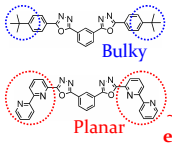
Orientation can also be controlled actively by intermolecular hydrogen bonds.

D. Yokoyama *et al.*, Adv. Funct. Mater. **21**, 1375 (2011)

3. Effects on electrical properties

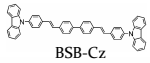


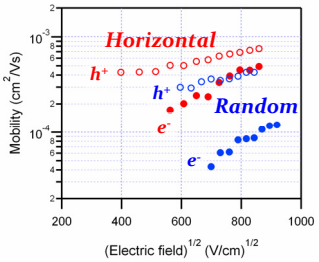
Control by terminal group



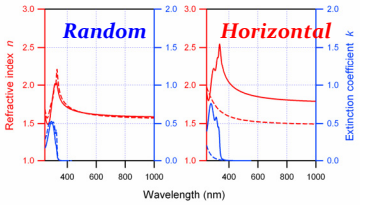
~30 times higher electron mobility

Control by substrate temp.





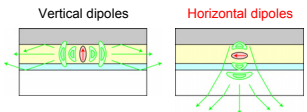
D. Yokoyama *et al.*, Adv. Funct. Mater. **20**, 381 (2010)



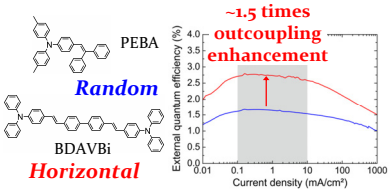
D. Yokoyama *et al.*, Appl. Phys. Lett. **95**, 243303 (2009)

Horizontal orientation can highly facilitate charge transport even in amorphous films.

4. Effects on optical properties

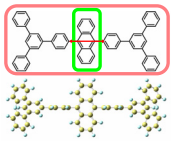


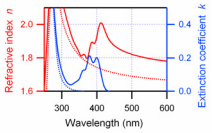
Dipole orientation of dopant emitter

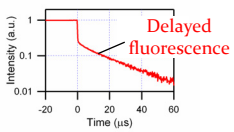


J. Frischeisen, *et al.*, *Org. Electron.* **12**, 809 (2011)

Dual enhancement in fluorescent OLEDs







Fluorescent OLED EQE >7%

S.-K. Kim *et al.*, J. Mater. Chem. **18**, 3376 (2008)

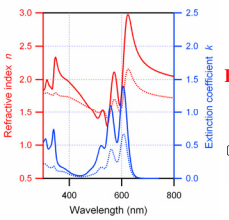
Outcoupling enhancement by dipole orientation × ***Singlet exciton generation via T-T annihilation***

Dual enhancement in extremely high-efficiency fluorescent OLEDs

D. Yokoyama *et al.*, *Appl. Phys. Lett.* **99**, 123303 (2011)

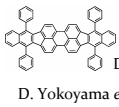
Horizontal orientation of transition dipole moments of emitting molecules significantly improves outcoupling efficiency of OLEDs.

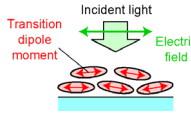
5. Application to OPVs



ITO/DBP (20 nm)/C_{70} (40 nm) /BCP (10 nm)/Al → **PCE >4%**

Horizontally oriented amorphous donor





Horizontal orientation of amorphous materials can be effectively used also for OPVs.

D. Yokoyama *et al.*, *Sol. Energy Mater. Sol. Cells.* **98**, 472 (2012)