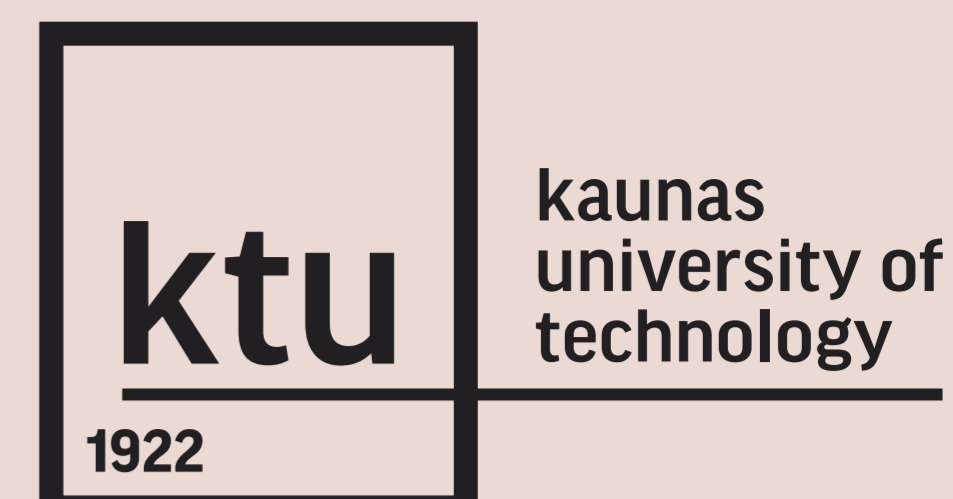


WET PROCESS FEASIBLE NOVEL FLUORENE-BASED MOLECULAR HOLE TRANSPORTING LAYER FOR PHOSPHORESCENT ORGANIC LIGHT EMITTING DIODES



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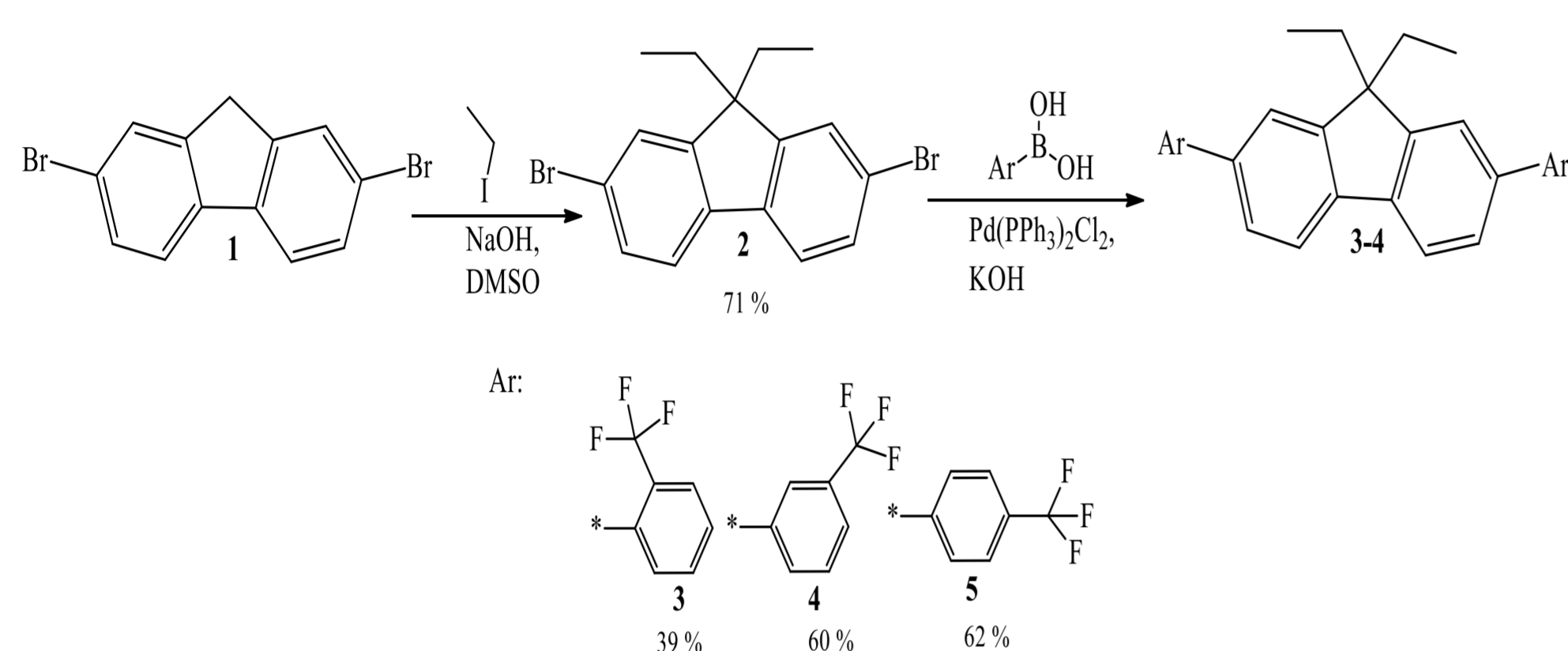
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Introduction

Organic light emitting diodes (OLEDs) are widely used in high-quality displays and show great potential lighting because of their superior characteristics. OLED possesses significant features for flat-panel display applications such as; self-emitting property, high luminous efficacy, full-color ability, wide viewing angle, high contrast, low power consumption, low weight, potentially large area, color displays, and flexibility [8–10]. These versatile features create rapid adaptability of OLED technology in consumer products. Performance improvement is one of the main reasons attributing towards effective adaptability. Whilst effective carrier recombination is an important strategy to improve the device performance.

Mainly two approaches are attributed to the fabrication of OLEDs, i.e. dry and wet processes. In the former approach, all the layers are deposited by thermal evaporation while in the wet process, layers are deposited by spin coating or else. The latter approach is feasible for commercial profit and enables large-area roll-to-roll fabrication. The molecular structure design and synthetic approaches of hole transporting materials, host materials, emissive materials, and electron transporting materials play a crucial role in the performance of OLEDs.

Synthesis



Scheme : Schematic illustration of synthesis fluorene type HTMs, 3, 4, and 5.

Thermal Properties

Compound	T _d	T _g	T _m	T _{cr}
3	248	17	144	-
4	252	-	142	106
5	255	-	138, 178	121, 159

When the derivative 5 was heated during the DSC experiment, two endothermic peaks due to melting were observed at 138 °C and at 178 °C. When the melt sample was cooled down, crystallizations of the two crystalline modifications were observed correspondingly at 121 °C and at 159 °C to form the same crystals, which were obtained by crystallization from solution.

Theoretical Calculations

Calculated frontier molecular energy levels by using B3lyp/631g(d,p)

Materials	HOMO (eV)	LUMO (eV)	E _g (eV)	ES ₁ (DCM) (eV)	ET ₁ (DCM) (eV)
Compound 3	-5.69	-1.32	4.37	4.36	3.32
Compound 4	-5.75	-1.58	4.17	4.16	3.17
Compound 5	-5.81	-1.71	4.10	4.10	3.13

To study the correlation between the electronic structure and photophysical properties of the compounds theoretical calculation were performed by using density functional theory at B3LYP/6-31G (d,p) level.

Properties of compounds 3-5

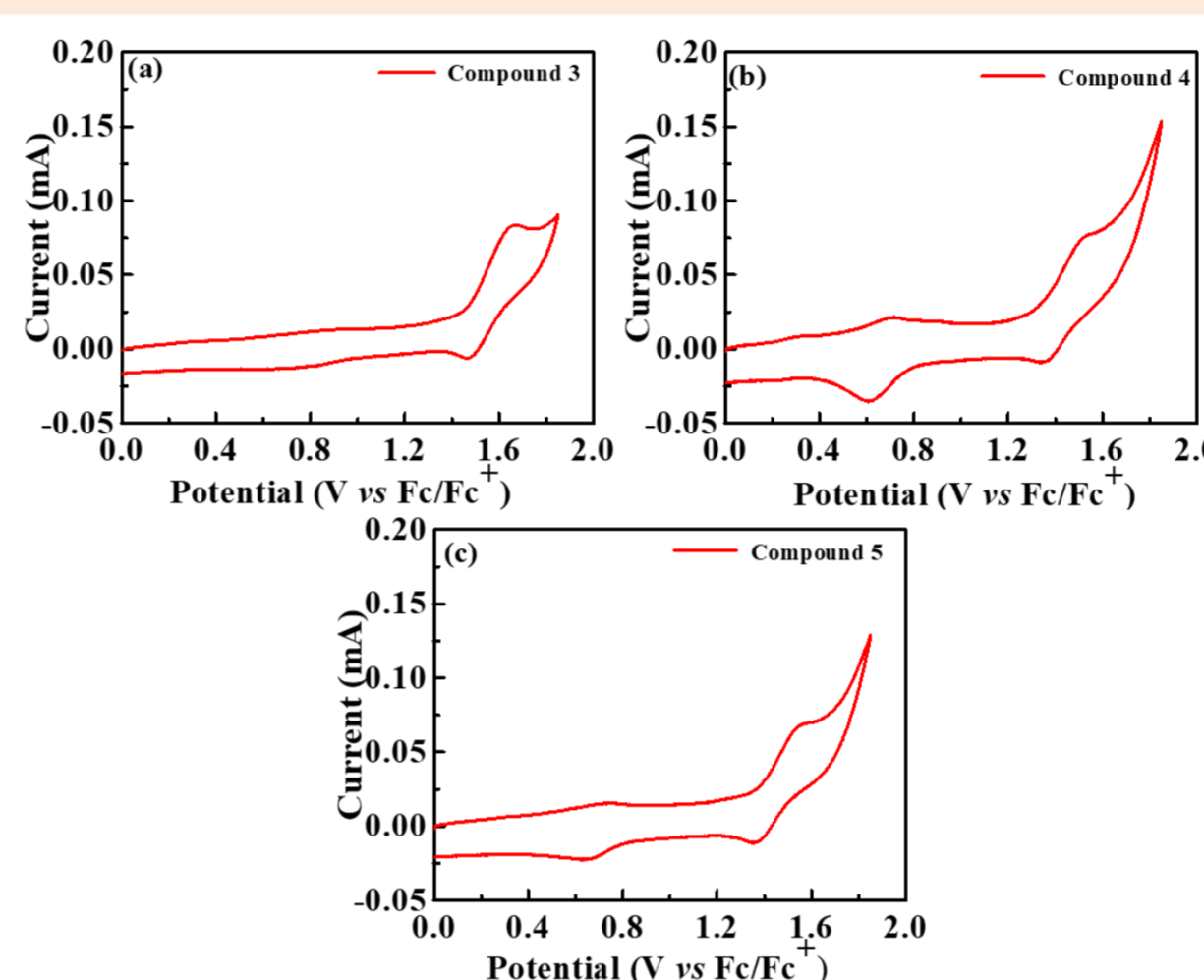


Figure 1. Cyclic voltammetric scans of the hole transporting materials 3, 4 and 5

All the materials showed more positive oxidation potential compared with ferrocene, displaying facile deletion of electrons from the molecule. The HOMO energy calculated from the estimated oxidation potentials. The calculated HOMO levels are 6.36, 6.24, and 6.26 eV for HTM 3, 4 and 5. From the HOMO level and optical energy band gap, we calculated LUMO levels. The obtained LUMO levels are 2.70, 2.73, and 2.88 eV respectively.

Ionization Potentials

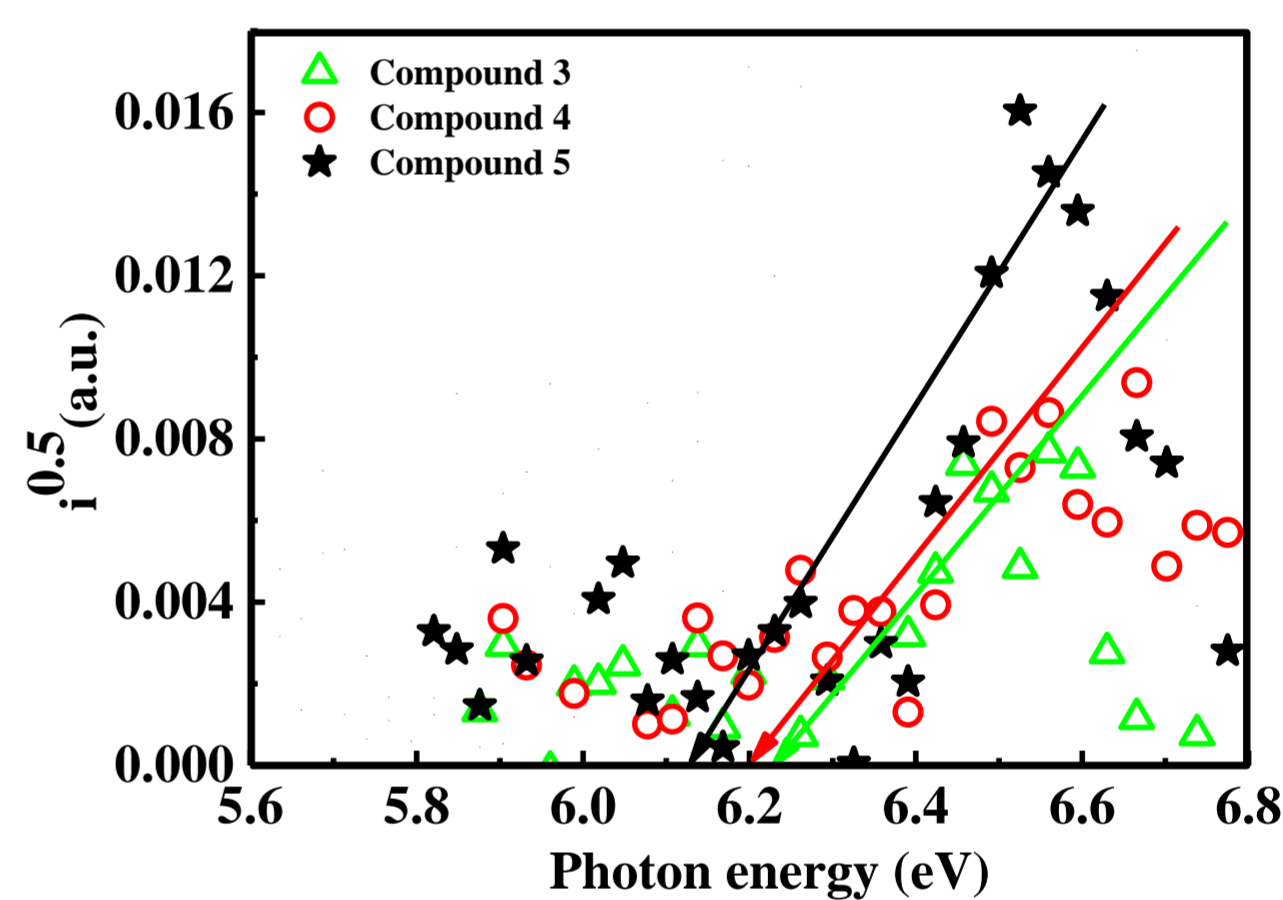


Figure 2. Electron photoemission spectra of Compound 3, 4 and 5

OLED characterisation

EL characteristics of the OLEDs fabricated using newly synthesized hole transporting materials

HTL	Solvent	OV (V)	PE _{100/1000/10000/Max} (lm/W)	CE _{100/1000/10000/Max} (cd/A)	EQE _{100/1000/10000/Max} (%)	CIE _{xy} coordinates	Max. Lum. (cd m ⁻²)
3	THF	6.2/8/-	13.4/7.3/-/14.6	26.5/18.5/-/27.9	10.2/-/10.8	(0.53, 0.47) - / -	4114
3	O-Xylene	5.4/7.2/10.2	14.8/8.5/2.7/23.1	25.4/19.4/8.9/29.4	7.7/5.9/2.7/9.0	(0.49, 0.51) / (0.49, 0.51) / (0.49, 0.51)	12120
4	THF	7.7/9.3/-	14.7/8.0/-/16.0	35.8/23.7/-/38.2	12.9/8.5/-/13.7	(0.52, 0.47) / (0.52, 0.47) -	8213
4	O-Xylene	5.4/7.3/10	14.0/8.6/3.9/22.8	24.1/20/12.5/29.2	7.4/6.1/3.8/9.0	(0.49, 0.51) / (0.49, 0.51) / (0.49, 0.51)	16700
5	THF	6.0/7.6/-	15.7/8.5/-/16.0	30.2/20.4/-/30.6	11.6/7.8/-/11.7	(0.53, 0.47) / (0.53, 0.47) -	6675
5	O-Xylene	5.5/7.5/10.5	16.6/9.2/3.6/27.9	29.3/22.0/12.1/35.7	9.0/6.7/3.7/10.9	(0.49, 0.51) / (0.49, 0.51) / (0.49, 0.51)	14800
NPB	THF	6.7/7.9/11.8	13.3/11.3/3.3/16.1	28.3/28.3/12.4/36.0	12.4/11.1/-/15.8	(0.53, 0.47) / (0.53, 0.47) -	10940
NPB	O-Xylene	5.5/7.5/10.4	14.1/8.3/3.5/20.3	24.8/19.7/11.4/25.4	7.6/6.0/3.5/8.0	(0.49, 0.51) / (0.49, 0.51) / (0.49, 0.51)	14540

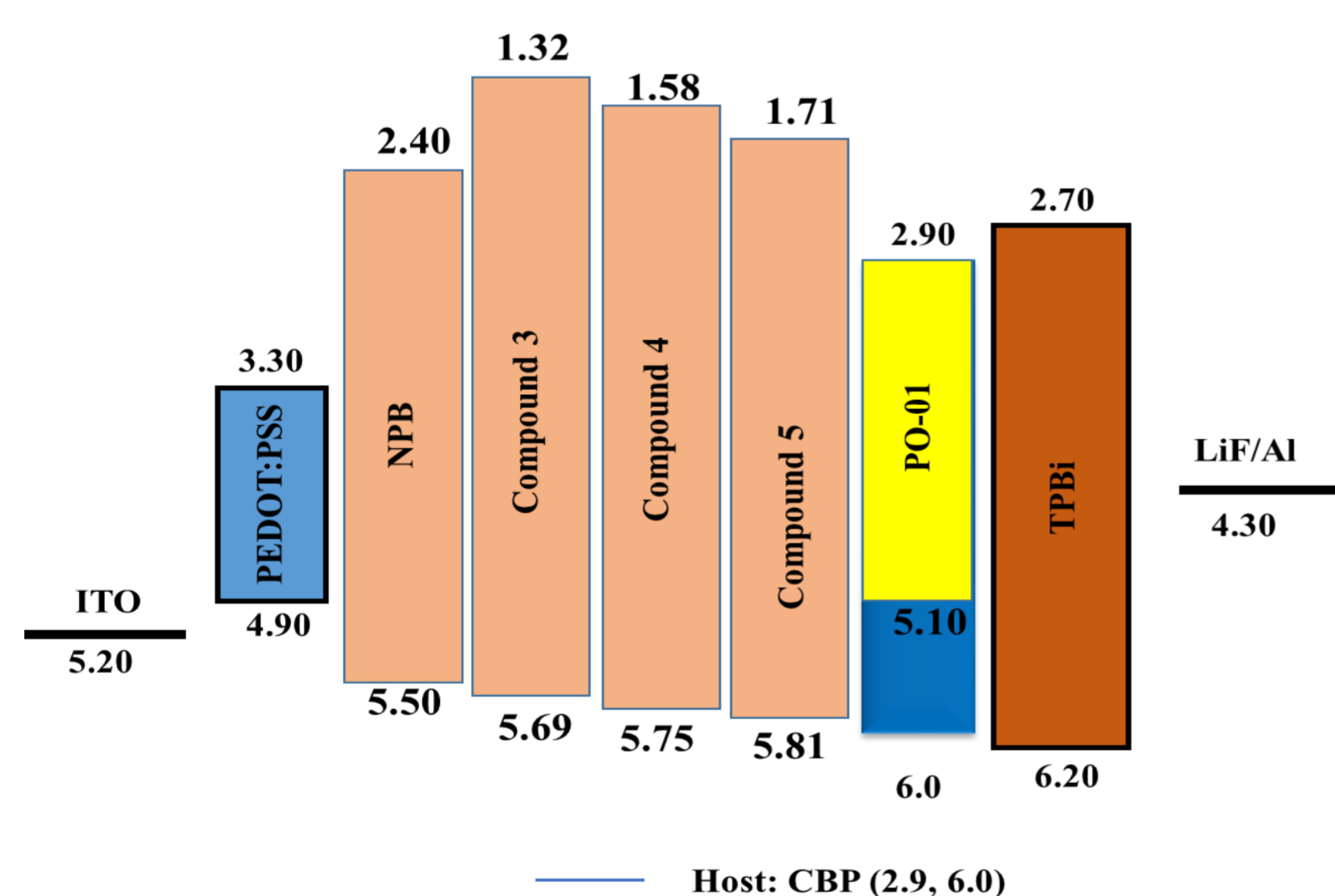


Figure 3. Schematic energy level diagram of OLED devices utilizing novel hole transporting materials.

Conclusions

In summary, novel fluorene based hole transporting materials were designed and developed for OLED application. Further, HTL material were studied with different solvents, THF and a low polar solvent *o*-Xylene. The selection of solvents was aimed to check the polarity of solvents influencing the device performance. Among the three materials, material-5 showed crystallization after spin coating, which was confirmed by morphological studies. By dissolving HTM in THF, results in improving the current efficiency increased from 23.3 to 35.8 cd/A at 100 cd/m², an increment of 54% by substituting the conventional HTM *N,N'*-di(1-naphthyl)-*N,N'*-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB), with the molecule 4 counterpart. Molecules 3 and 5 also showed a competing performance in the devices. The high triplet energy, electron blocking capability, the high ionization potential of the molecules improved the carrier confinement in the emissive layer and the device performance. When using *o*-Xylene, the PE and CE of the devices showed improvement. Especially, the maximum PE of all the devices improved compared to the devices which fabricated by using THF. The maximum PEs improved from 14.6, 16.0, 16.0, and 16.1 lm/W to 23.1, 22.8, 27.9, and 20.3 lm/W respectively for 3, 4, 5, and NPB by changing the solvent to *o*-Xylene. EQE decreased in *o*-Xylene based devices, which may be due to the unbalanced electron-hole injection.

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