Solution-processable organic semiconductors based on anthracene as main components of active layers in OLEDs: Design, synthesis and application

Veroniki P. Vidali[1], Maria Vasilopoulou[1], Dimitra Niakoula[1], Anna Kapella[1,2], Apostolos Verykios[1], Evangelos T. Georgas[1], Stella Kennou[3], Daman R. Gautam[1], Evangelos Gogolides[1], Elias A. Couladouros[1,2], Panagiotis Argitis[1]

[1]Institute of Nanoscience & Nanotechnology, NCSR "Demokritos", Athens, Greece; [2]Chemical Laboratories, Agricultural University of Athens, Greece; [3]Department of Chemical Engineering, University of Patras, Patras, Greece . Email: v.vidali@inn.demokritos.gr

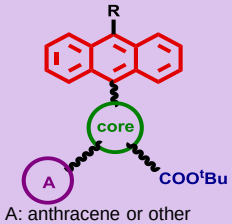
Introduction

Well-defined, monomolecular amorphous organic materials, based on polyaromatic compounds, have been receiving attention for the development of organic devices in the nanoscale with substantially enhanced performance and new functions. Moreover, in the case of OLEDs, solution-processability of such materials is highly desirable, since techniques, such as spin-coating, lower significantly the cost for the fabrication of the devices. Among polyaromatic molecules, anthracene exhibits interesting photoluminescence, electroluminescence and excellent electrochemical properties. Indeed, anthracene derivatives have been extensively studied in OLEDs, either as emitting or charge transport materials. However, most of them were synthesized by metal-catalyzed reactions leading mainly to symmetric structures, where the anthracene unit is directly connected to other aromatic or conjugated systems. Moreover, its high crystallization and sublimation tendency necessitates efficient structure modifications in order to control these properties. Herein, we present a different design strategy and synthesis of a new class of solution-processable small molecules based on anthracene for incorporation in films. Results of studies of their properties related to film formation (solubility, sublimation and Tg), as well as their evaluation as active layer materials in organic light emitting devices are also shown.

Results & Discussion

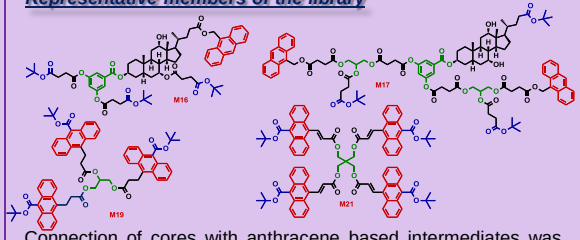
Design of new molecules – Control of film properties

Attachment of anthracene units to a planar or non-planar cores (e.g. resorcinol derivatives, glycerol, pentaerythritol) allowed ease of preparation, control of molecular architecture and high variety of structures. Tert-butyl ester group was introduced in the structures to allow patterning. Film-forming properties were thus controlled and stable, amorphous films were obtained.



A: anthracene or other polycarbocycle

Representative members of the library



Connection of cores with anthracene based intermediates was based on esterification reactions.

Solubility & Thermal properties studies

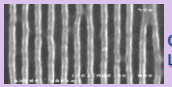
Sublimation temperatures obtained are proper for processing of films. Evaluation of Tg showed that the compounds form molecular glasses, which is desirable for the formation of amorphous films.

Compound[(a)]	Sublimation (°C)	Tg (°C) [(b)]
M16	160	54 (64)
M17	110	37 (57)
M19	150	30 (80)
M21	150	57 (88)

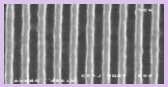
[(a)]All compounds were soluble in MIBK (4% w/w). [(b)]Tg in film *obtained by OPTI method*

A patterning example – EUV evaluation

Solution-processable anthracenes blended with suitable PAGs, have provided sub-40 nm features, as shown from EUV evaluation.[1] Example shown is for **M17**. Similar results were obtained with M21.[3]

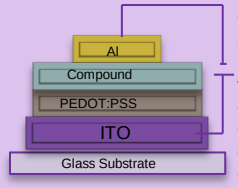


CD 32.5 nm
LER=2.6±0.5



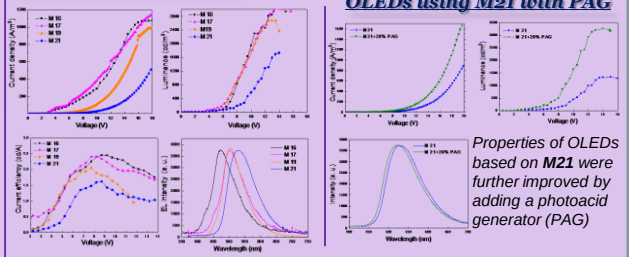
CD 37.7 nm
LER=2.4± 0.5

Device characterization of OLEDs with the structure ITO/PEDOT-PSS/M resist/Al



The new compounds were evaluated as emissive layers in OLEDs of conventional architecture. are depicted below. OLEDs based on these compounds exhibited very promissing operational characteristics (current density, current efficiency, luminance), while emission of different colour was observed in each case.

OLEDs using M21 with PAG



*Properties of OLEDs based on **M21** were further improved by adding a photoacid generator (PAG)*

The new molecules exhibit tunable energy levels depending on their structure.
This property renders them appropriate for application in a broad range of optoelectronic devices.

Conclusions

A design and synthetic strategy for the development of a new class of solution-processable well-defined anthracene-based molecules for incorporation in films was introduced. Compounds designed with this strategy exhibited enhanced properties related to the film via control of the molecular architecture and they led to stable, amorphous and patternable films used succesfully as emissive layers in OLEDs.

References

1. G. Vannuffel , D. Djian, S. Tedesco, D. Niakoula, P. Argitis, V. P. Vidali, E. A. Couladouros, H. Solak Proceedings of SPIE-The International Society for Optical Engineering 6519 (part 2) 2007, 651949.
2. P. Argitis, E. Gogolides, D. Niakoula, V.P. Vidali, E.A. Couladouros, D.R. Gautam, US patent: 8247158, 21/8/2012.
3. P. Argitis,,, , D. Niakoula, A. M. Douvas, E. Gogolides, I. Raptis, *Int. J. Nanotechnol.* 2009, *6(1)*, 71.