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New Functional Anthracene Based Liquid Crystals Towards Organic Optoelectronic Device Applications

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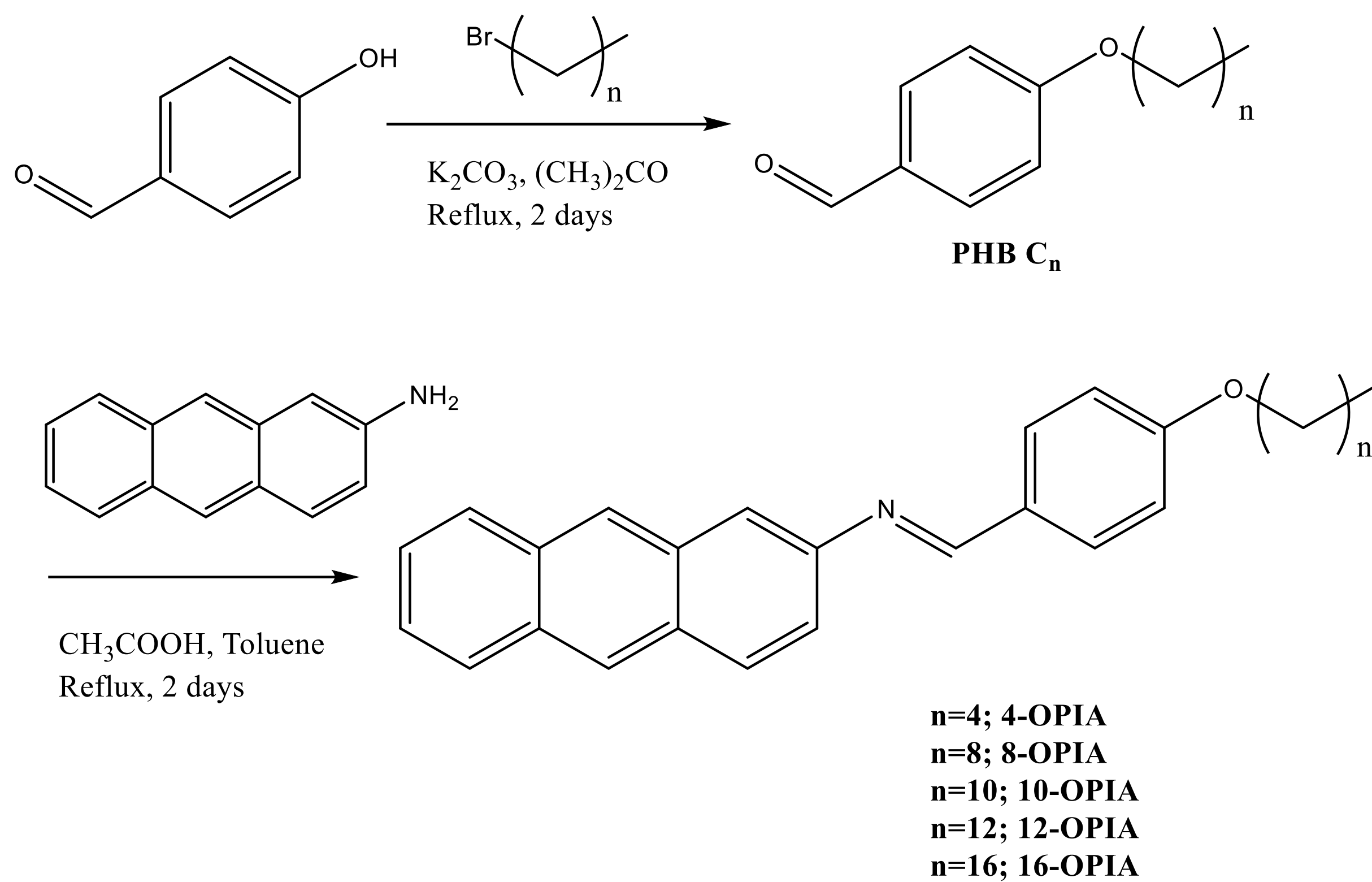
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ABSTRACT

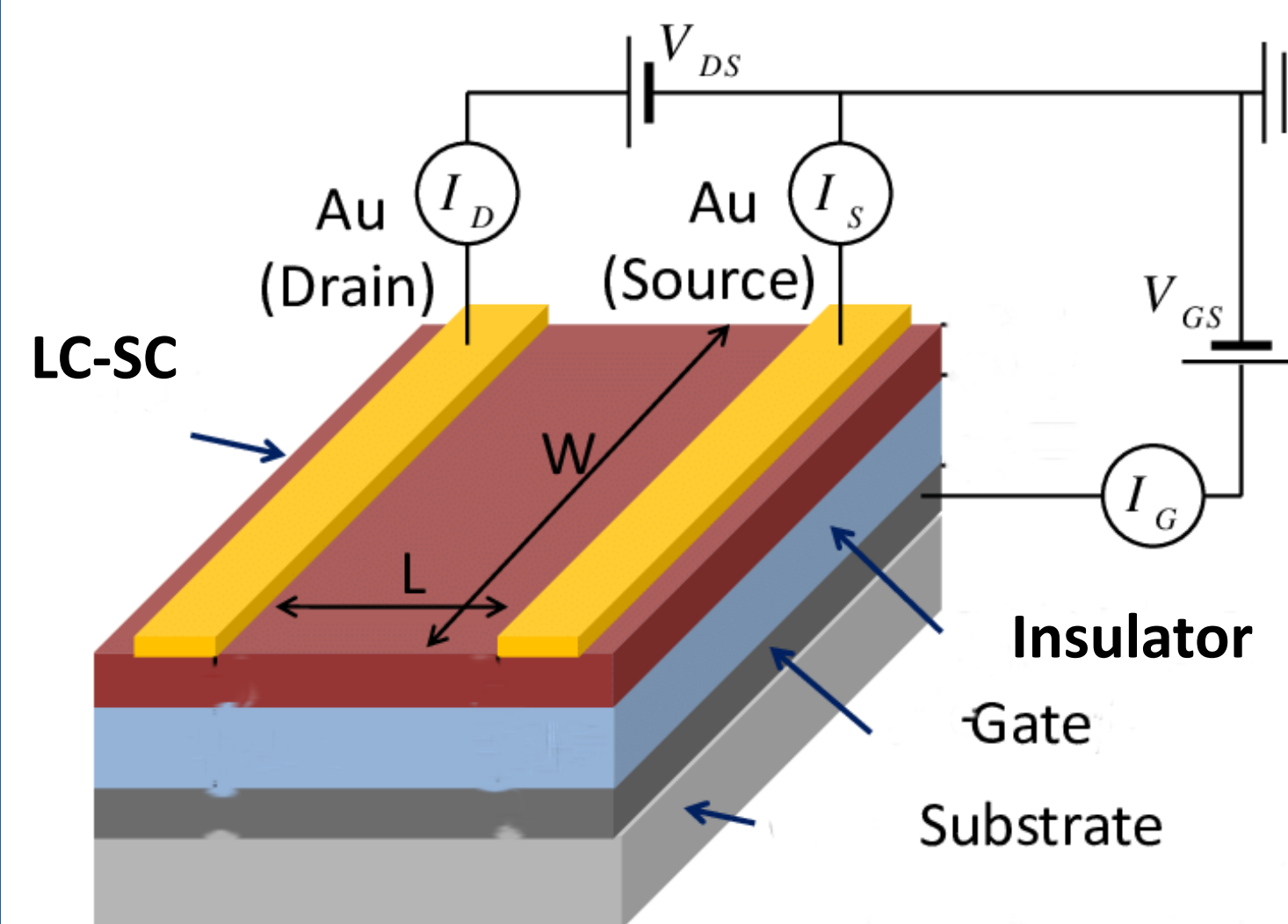
This study focuses on the development of new multifunctional mesogenic semi-conducting (LC-SC) materials based on 2-amino anthracene and para-hydroxybenzaldehyde (n-OPIA with n=4, 8, 10, 12 and 16). Each material contains a central rigid phenyl-anthracene core, and one terminal flexible alkyloxy chain with different length. These materials are based on the concept of liquid crystal (LC) materials featuring facile processability, highly ordered alignment and effective charge transport. Their thermal behaviors are performed by means of differential scanning calorimetry and polarized optical microscopy, and showed differences on mesomorphic behaviors with respect to the length of the terminal alkyloxy chain. The frontier molecular energy levels were studied by optical spectroscopy and cyclic voltammetry and compared to values obtained via ab initio DFT calculations. The photoexcitation ($\lambda = 455$ nm) of LC Field-Effect Transistors (LC-FETs) based n-OPIA films revealed efficient photo-responsive characteristics in relation to alignment due to alkoxy chain length, indicating their promising potential applications in multifunctional integrated devices.

SYNTHESIS



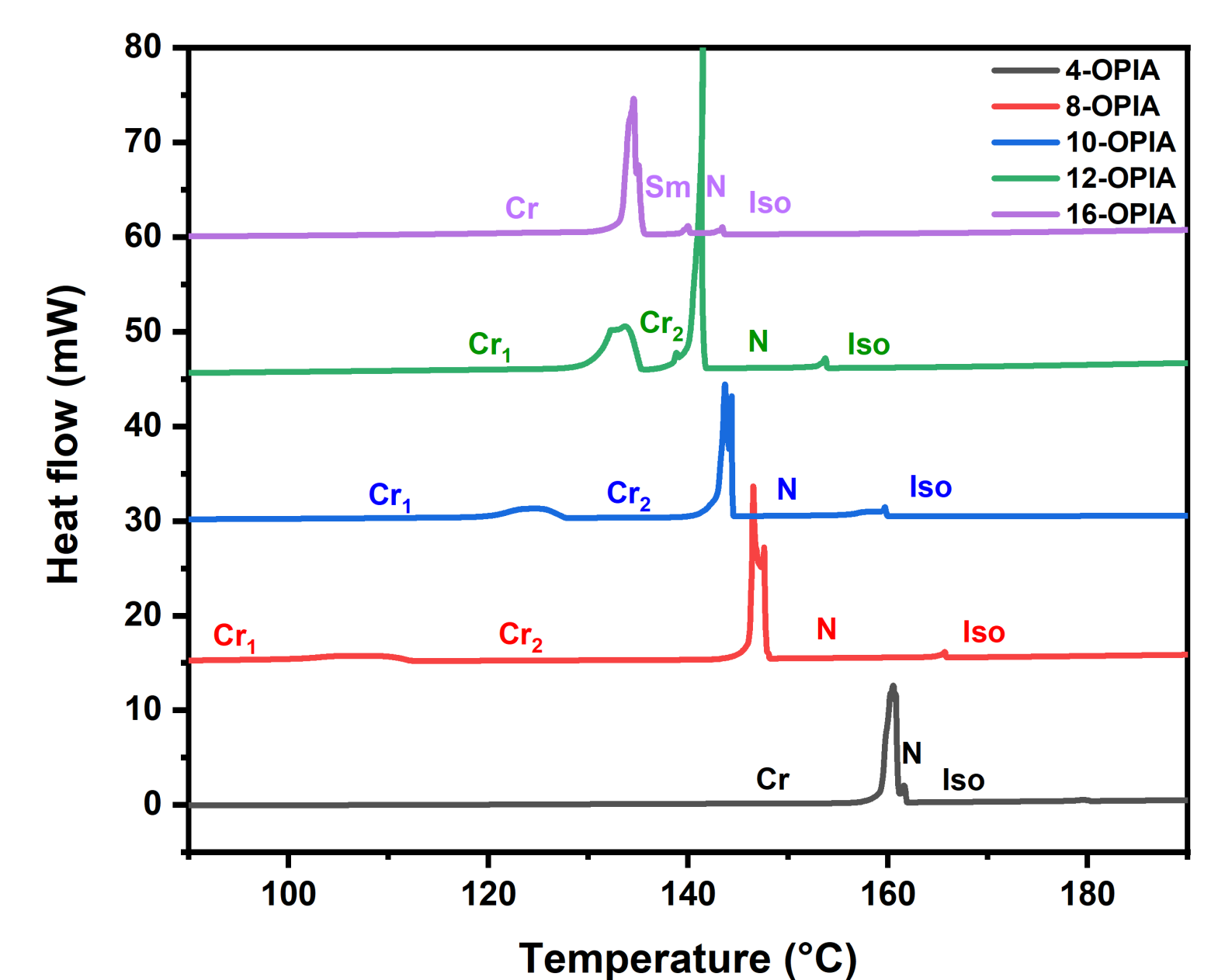
Synthesis of our n-OPIA liquid crystal semi-conducting materials (LC-SC)

SCHEMATIC OF LC-FETS



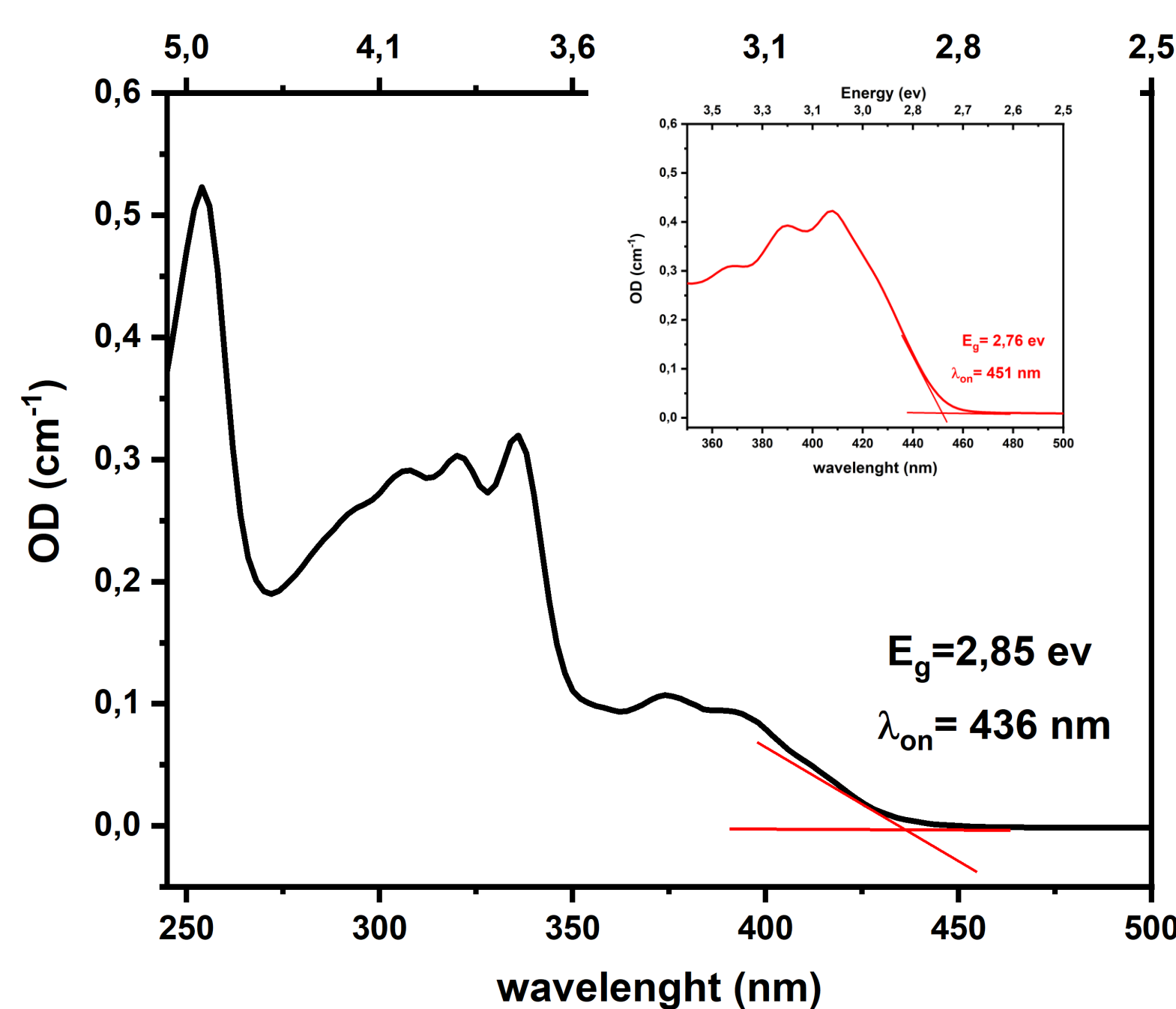
Schematic of LC-FETs characterization device

MESOMORPHIC BEHAVIORS

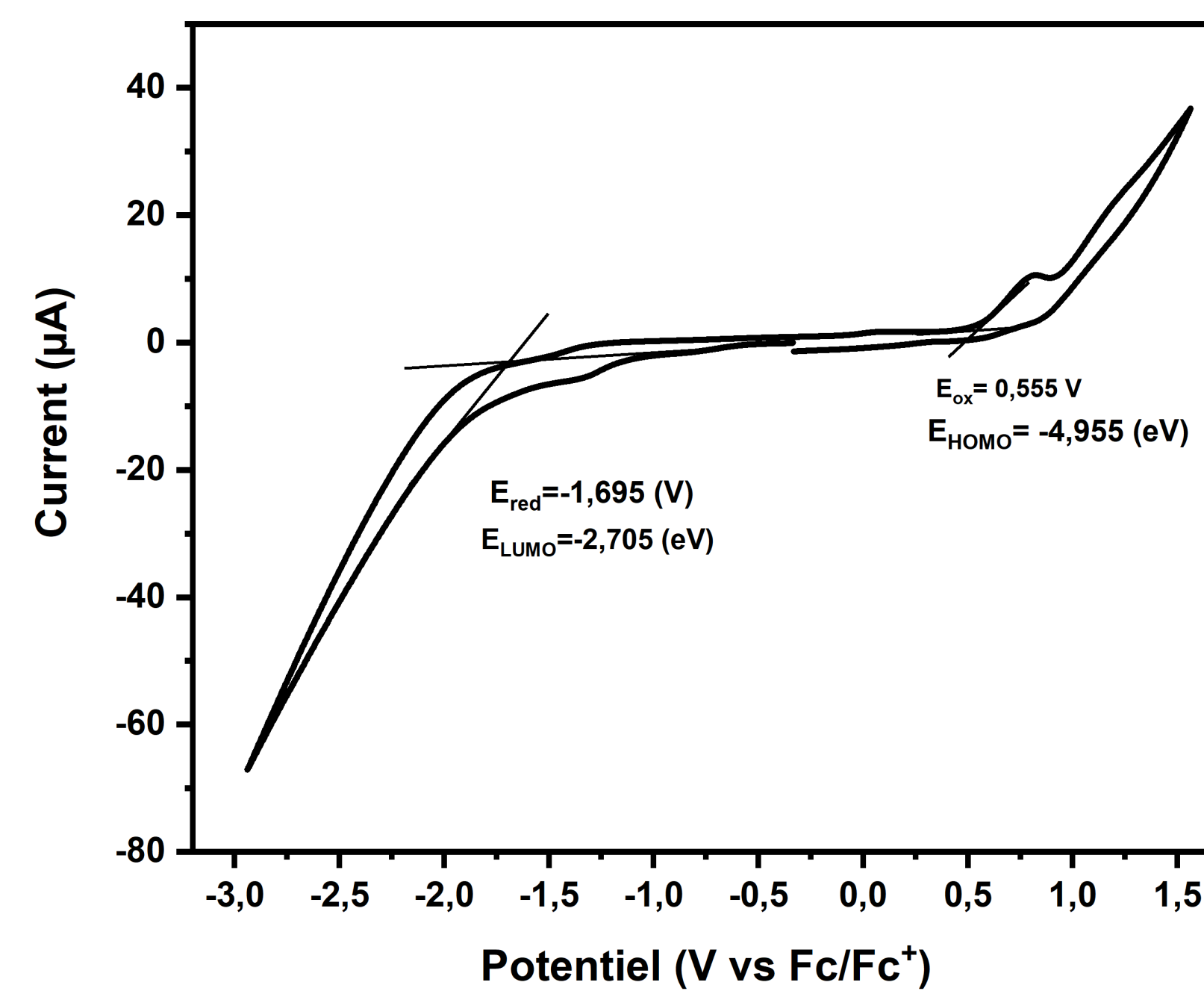


DSC thermograms of n-OPIA on cooling with a rate of 10°C/min showed differences on mesomorphic behaviors with respect to the length of the terminal alkyloxy chain and the crystallization temperature is inversely proportional to the increase in alkoxy chain length.

EXPERIMENTAL RESULTS



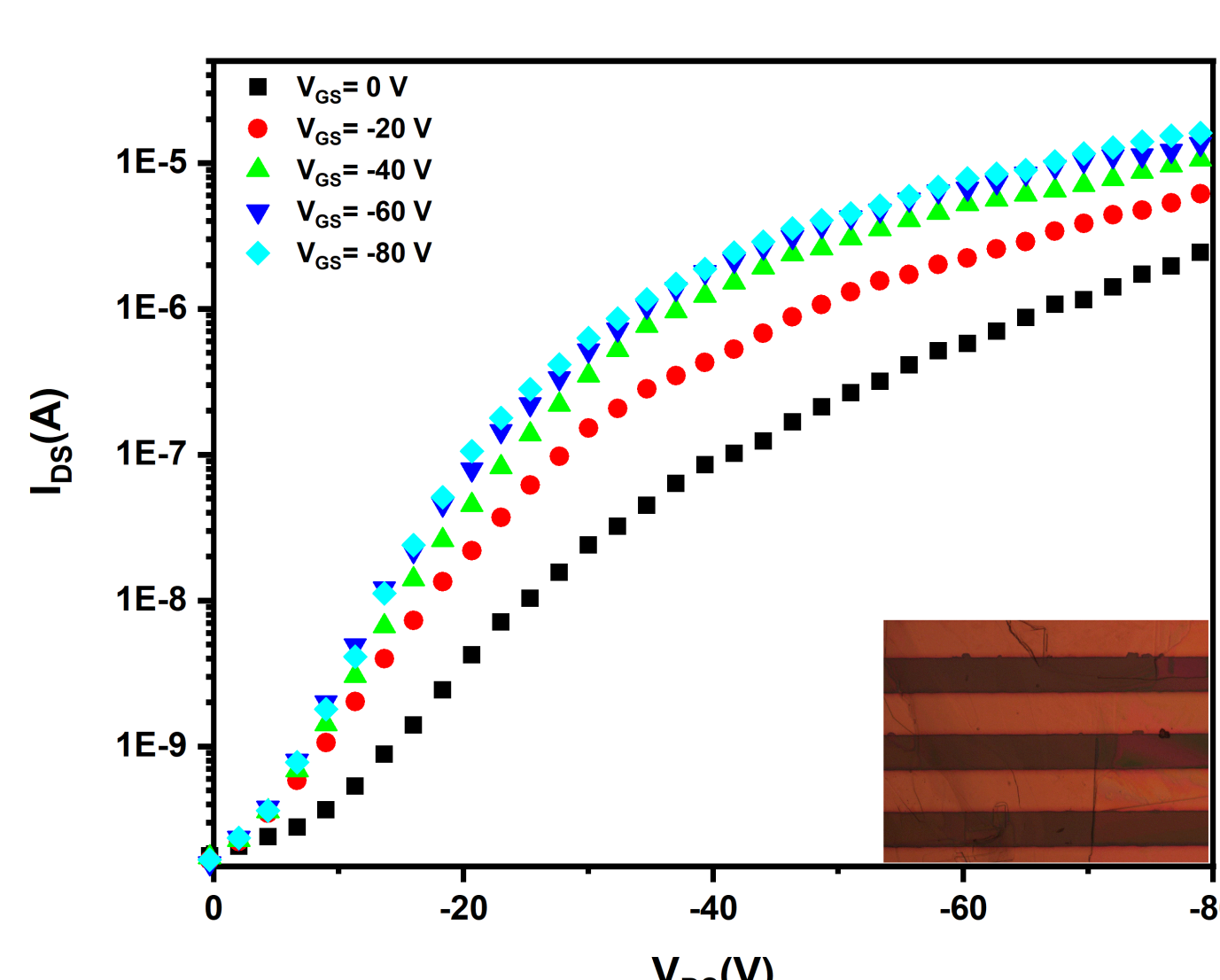
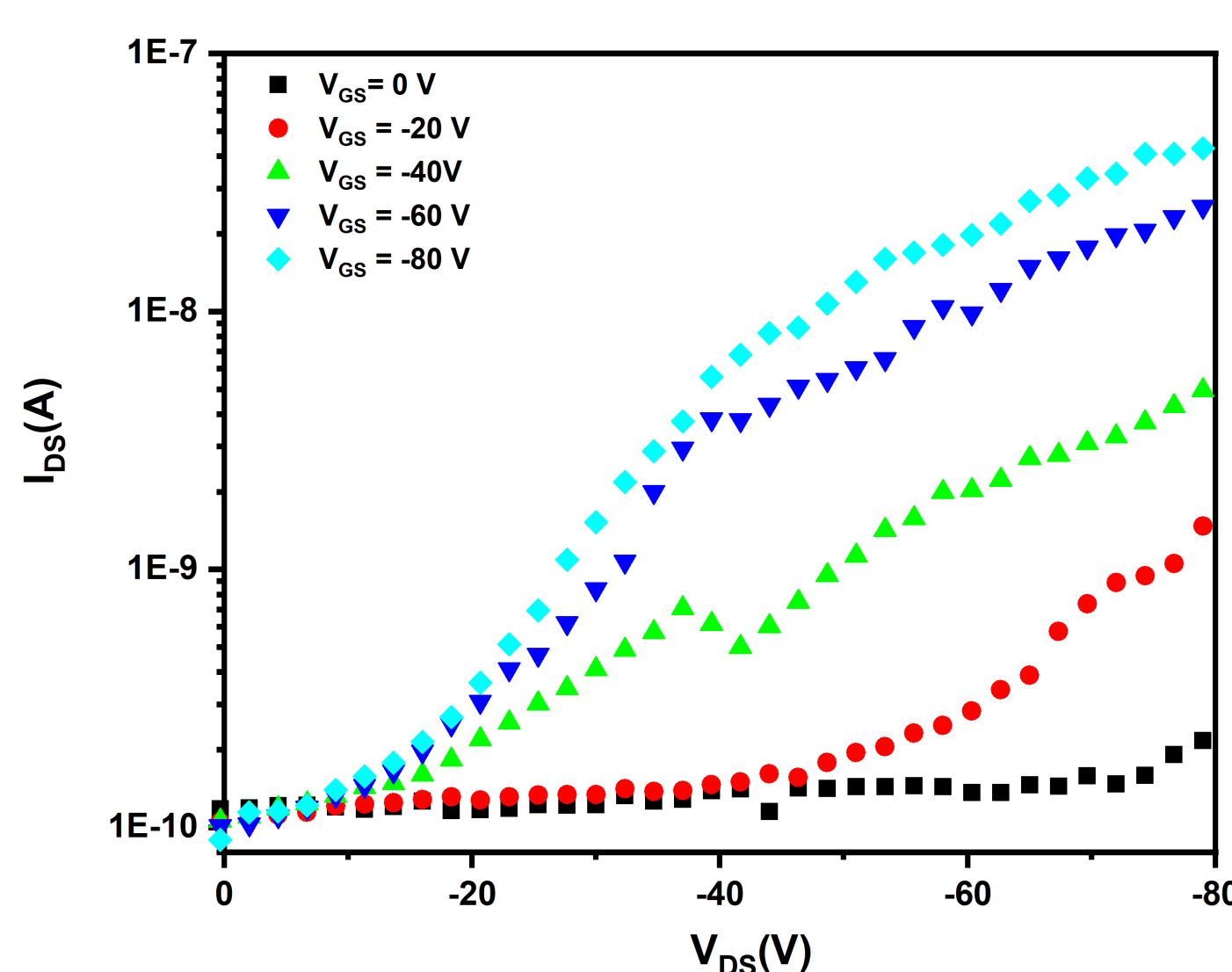
Example of optical absorption spectrum obtained for 8-OPIA (10^{-5} M solution in dichloromethane). Inset: absorption for drop-casted thin film of 8-OPIA (0.5% wt. in chlorobenzene) on quartz substrate



Example of normalised cyclic voltammetry data obtained for 8-OPIA (2mmol) in 0.1TBAPF₆ in DCM, degassed with Ar (20 minutes) at 50mV/s versus Fc/Fc⁺.

| | $E_{\text{HOMO-DFT}}$ (eV) | $E_{\text{LUMO-DFT}}$ (eV) | E_g (HOMO-LUMO) DFT (eV) | $E_{\text{HOMO-CV}}$ (eV) | $E_{\text{LUMO-CV}}$ (eV) | E_g (HOMO-LUMO) CV (eV) | $\lambda_{\text{max-DFT}}$ (nm) | $E_g^{\lambda_{\text{max}}}$ DFT (eV) | E_g -UV-film (eV) | $\lambda_{\text{max-UV-film}}$ (nm) |
|---------|----------------------------|----------------------------|----------------------------|---------------------------|---------------------------|---------------------------|---------------------------------|---------------------------------------|---------------------|-------------------------------------|
| 4-OPIA | -5,27544 | -2,02504 | 3,25504 | -5.03 | -2.32 | 2,71 | 419,81 | 2,953 | 2,86 | 434 |
| 8-OPIA | -5,28034 | -2,03102 | 3,24932 | -4.95 | -2.7 | 2,25 | 418,32 | 2,963 | 2,76 | 451 |
| 10-OPIA | -5,27381 | -2,02422 | 3,24959 | -5.18 | -2.46 | 2,72 | 419,49 | 2,955 | 2,74 | 453 |
| 12-OPIA | -5,27462 | -2,02477 | 3,24985 | -5.01 | -2.62 | 2,39 | 419,31 | 2,956 | 2,76 | 449 |
| 16-OPIA | -5,27354 | -2,02368 | 3,24986 | -5.28 | -2.61 | 2,67 | 419,46 | 2,955 | 2,74 | 453 |

Frontier molecular energy levels properties for our n-OPIA materials obtained from optical spectroscopy and cyclic voltammetry experiments, and compared to values obtained via ab initio DFT calculations which showed HOMO of n-OPIA align well with gold, that allowed us to use this classic material for electric contacts in order to create a P-type transistor.



Output characteristics in dark (left) and under illumination (right) ($\lambda = 455$ nm) at incident power of 1 mW/cm² of bottom gate FET prepared with drop-casted 8-OPIA film (thickness of about 600 nm). Inset: microscope capture (in polarized light) of the inter-digitated electrode of 8-OPIA-FET (L = 50 µm, W=18mm) used for measurements.

| n-OPIA | μ_{hole} (cm ² / (V s)) | $I_{\text{ON}}/I_{\text{OFF}}$ | V_{th} (V) |
|-----------------------|-----------------------------------------------|--------------------------------|---------------------|
| 8-OPIA without light | 1.8×10^{-4} | 10 ³ | -53 |
| 8-OPIA with light | 1.9×10^{-3} | 35,4 | 8 |
| 10-OPIA without light | $1,8 \times 10^{-5}$ | 10 ² | -20 |
| 10-OPIA with light | 8×10^{-4} | 10 ² | 20 |
| 12-OPIA without light | 1.06×10^{-4} | 1460 | -10 |
| 12-OPIA with light | 9.8×10^{-3} | 32,3 | 17 |
| 16-OPIA without light | $1,9 \times 10^{-5}$ | 2300 | -62 |
| 16-OPIA with light | 1.5×10^{-4} | 1830 | 3 |

Relevant properties of charge transport without and with illumination ($\lambda = 455$ nm) at incident power of 1 mW/cm² of n-OPIA materials which exhibits reasonable field effect hole mobility in solution-processed thin film.

CONCLUSION

In summary :

- Novel homologous series of liquid crystal based phenyl-anthracene with different alkoxy chain length were synthesized and characterized.
- The thermal behaviors were performed by means of differential scanning calorimetry and polarized optical microscopy.
- Frontier molecular energy levels were studied by optical spectroscopy and cyclic voltammetry and compared to values obtained via ab initio DFT calculations.
- Efficient photo-responsive characteristics indicate their promising potential applications in multifunctional integrated optoelectronic device applications.

REFERENCES

1) Kondratenko, K.; Carlescu, I.; Danjou, P.-E.; Boussoualem, Y.; Simion, A.; Duponchel, B.; Blach, J. F.; Legrand, C.; Hurduc, N.; Daoudi, A. Novel Organic Semiconductors Based on 2-Amino-Anthracene: Synthesis, Charge Transport and Photo-Conductive Properties. Phys. Chem. Chem. Phys. 2021, 23 (25), 13885–13894. <https://doi.org/10.1039/D1CP01427G>.

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