Investigation of naphthalenediimide with phenothiazine as photoinduced charg-separating junctions

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Introduction

Photoinduced charge separating molecular systems are often key players in clean energy generation, such as organic photovoltaic devices.[1] These systems are usually composed of a heterojunction of an electron donor (D) and an electron acceptor (A). Naphthalene diimide (NDI) is a promising A-unit due to its relatively high electronic affinity and propensity for π-stacking.[2] On the other hand, phenothiazine dyes are excellent light absorbers and good electron donors.[3]

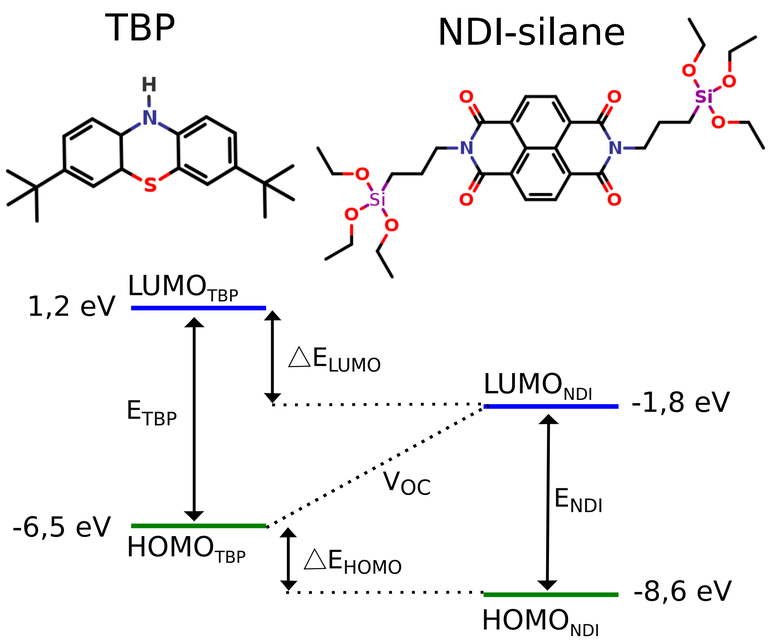

Figure 1: 2D representation of the TBP and NDI-silane and the energies of the HOMO and LUMO orbitals as calculated by the optimally tuned range separated hybrid (OT-RSH) functional in density functional theory (DFT).

In order to investigate junctions as D-A, we prepared and characterized optically, morphologically and electrically thin films of 3-triethoxysilylpropyl-1,4,5,8-naphthalenediimide (NDI-silane) with 3,7-diterc-butylphenothiazine (TBP).

Methodology

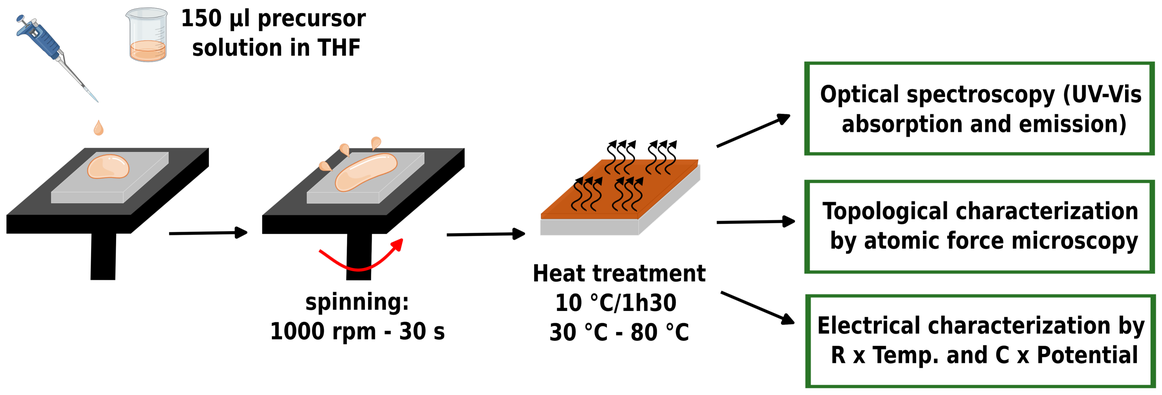

Figure 2: Schematic of the preparation and characterization of thin films of NDI-silane and 1:1 v/v TBP-NDI-silane.

Results & discussions

Thin films were prepared with an optimized thickness of 300-500 nm. Their optical spectroscopy showed absorption bands at 360 nm and 390 nm, and emission bands at 420 and 540 nm.

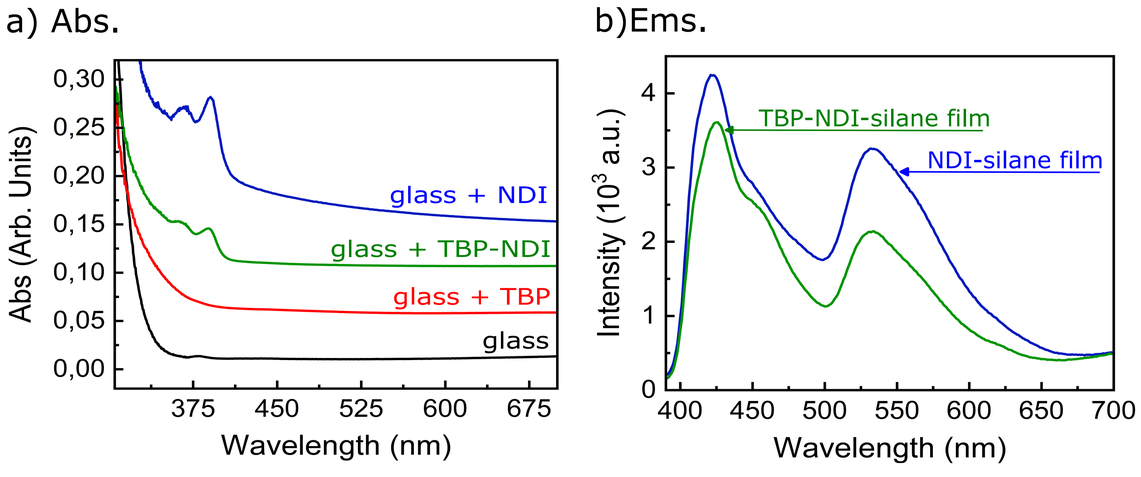

Figure 3: a) UV- Vis absorption spectra and b) emission spectra with excitation at 395 nm for thin films in glass substrates

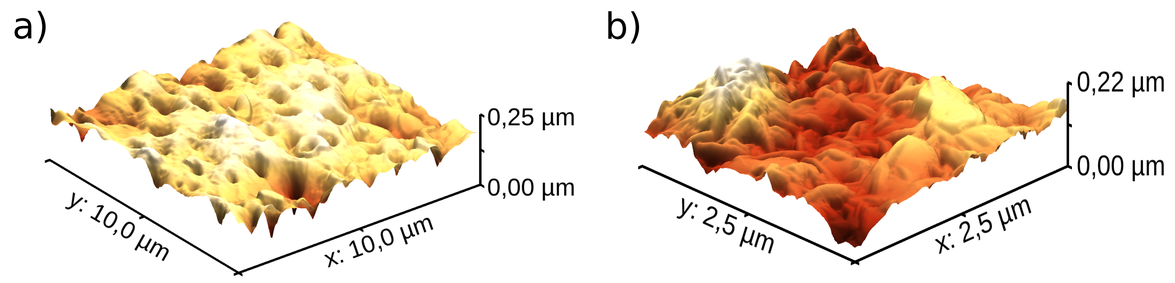

Figure 4: Topologies from atomic force microscopy of the a) NDI-silane and b) TBP-NDI-silane films

We observed a photo-conductivity effect with a difference in resistance of 1000 MΩ for the NDI-silane and around 50% for the TBP-NDI-silane.

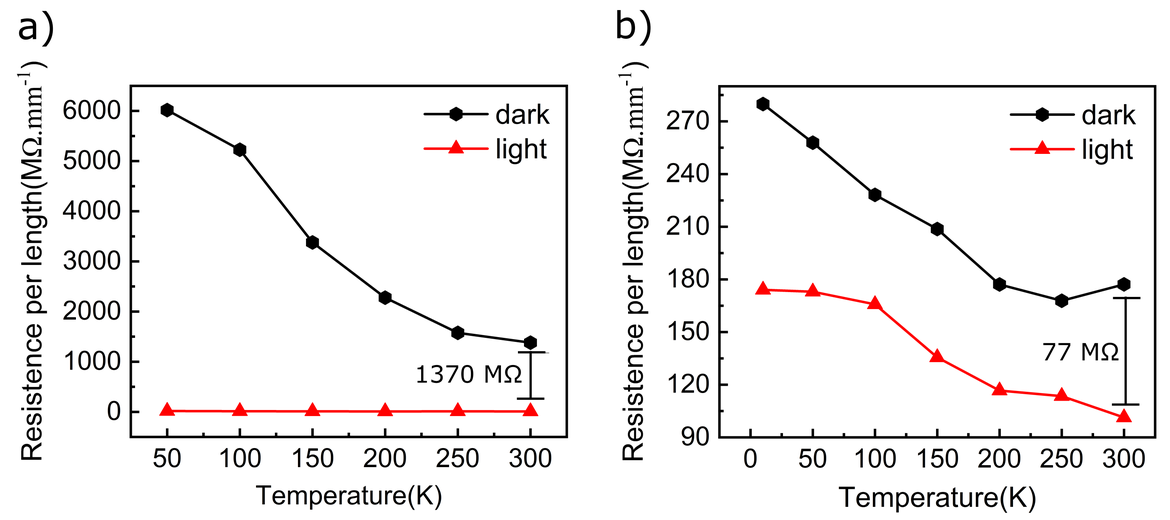

Figure 5: Resistance as a function of temperature with the system in the dark and under laser irradiation at $\lambda = 405$ nm of the (a) NDI-silane and (b) TBP-NDI-silane films.

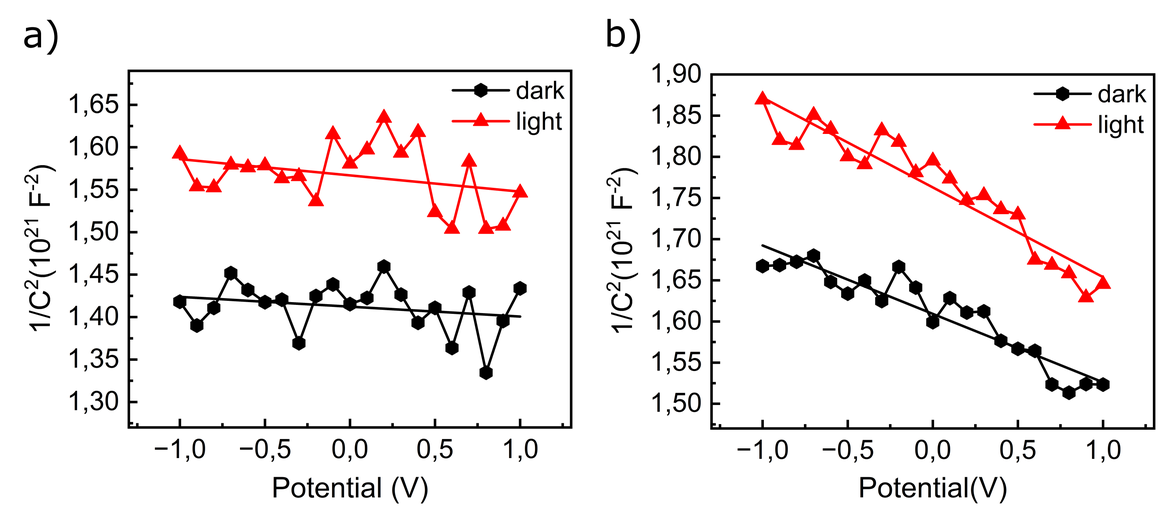

Figure 6: The inverse of the capacitance squared ($1/C^2$) as a function of potential at frequencies of a) 360 kHz and b) 960 kHz for the NDI-silane film with the system in the dark and under laser light

Conclusions & perspectives

- Thin films were prepared with good homogeneity and optimal thickness of 300-500 nm, significant absorbance in the UV and blue region.
- Both thin films showed a measurable photo-conductivity effect. In particular, the NDI-silane film showed an increase in the density of charge carriers in the presence of light.

Acknowledgements

R. G. A. acknowledges the FAPESP's scientific initiation program with the project 2021/07694-4. T. B. Q. acknowledges FAPESP for the young research program 2020/13466-1 and the PRH-ANP-UFABC program. M. T. E. acknowledges FAPESP grant 2022/11278-9. We are thankful to Prof. Álvaro Takeo Omori (UFABC) and Andreia J. O. Meira for the synthesis of the diterc-butylphenothiazine.

References

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