Nano Innovation 2021 Rome, 21-24 September Conference & Exhibition

Sustainable approaches to the synthesis and functionalization of phthalocyanines for optoelectronic applications

Laura Mancini[a], Gloria Zanotti[a], Anna Maria Paoletti[a], Patrizia Dolce[b]

a: Istituto di Struttura della Materia (ISM) - CNR, Via Salaria km 29.300, 00015 Monterotondo (Rm), Italy

b: Istituto di Struttura della Materia (ISM) - CNR, Area Industriale, 85050 Tito Scalo (Pz), Italy

laura.mancini@ism.cnr.it

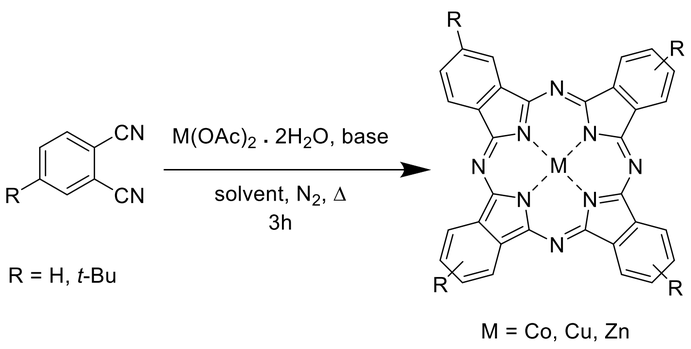
Introduction

Variously substituted phthalocyanines can be used as p-type molecular semiconductors in optoelectronic devices. In addition to maximizing the performance of the target technology it is desirable to develop materials using green synthetic approaches, possibly less expensive than those at the state of the art.

Goals:

- investigate alternative reaction conditions for environmentally and economically sustainable synthesis of metallophthalocyanines;
- investigate the role of several phthalocyanines as hole transport materials (HTMs) through preliminary measurements in perovskite solar cells;
- find viable alternatives to the use of expensive spiro-OMeTAD.

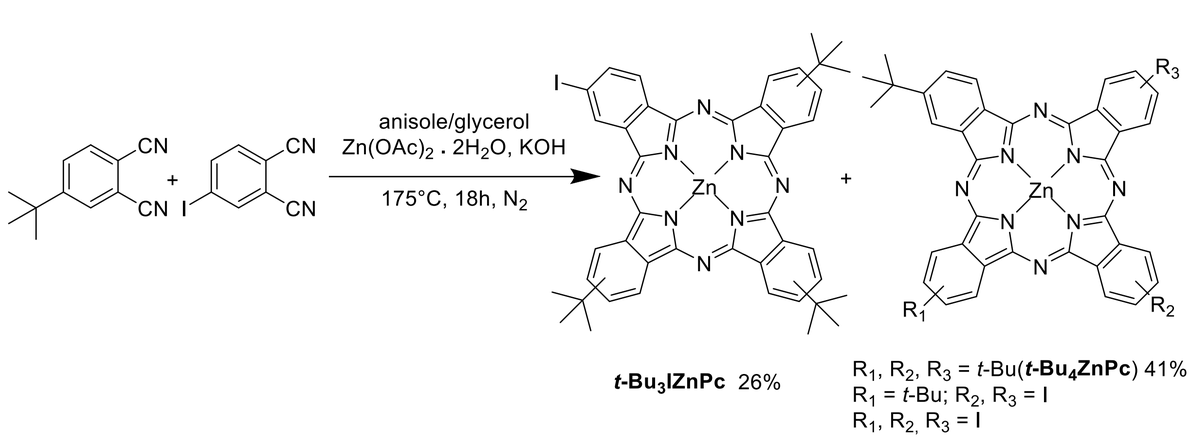
Synthetic pathway

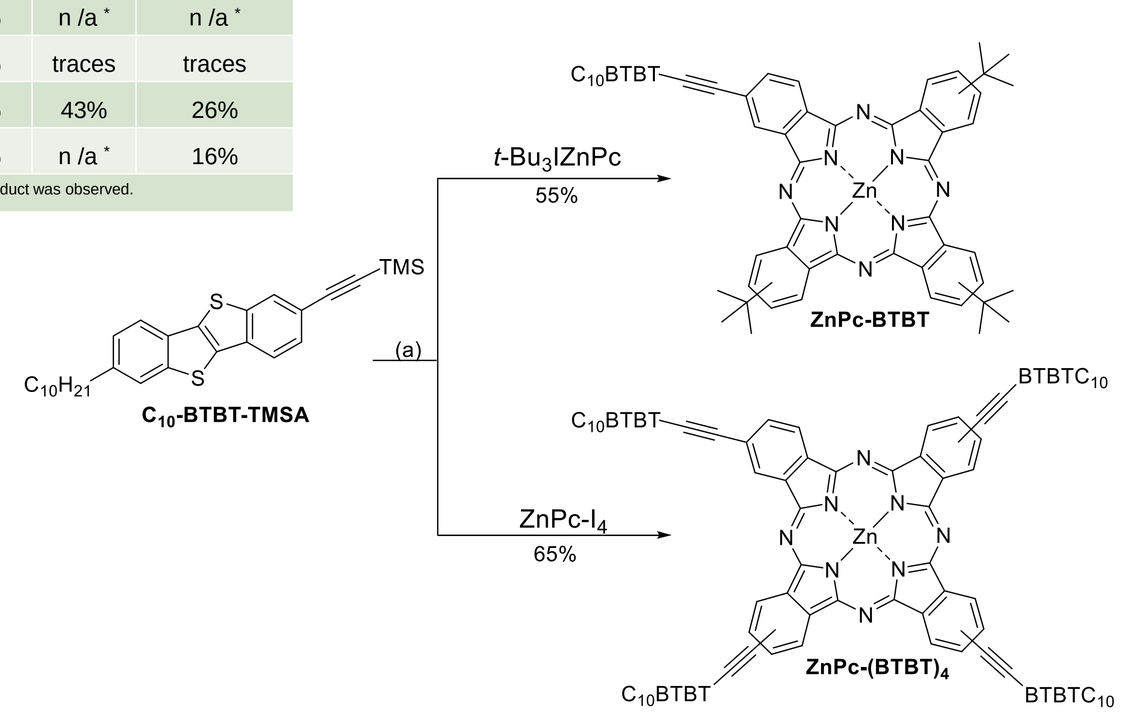


Product	DMAE-DBU	A-DBU	A-KOH	GA-KOH
CoPc	87%	72%	24%	37%
CuPc	83%	49%	76%	73%
ZnPc	75%	56%	n /a *	n /a *
t-Bu$_4$CoPc	62%	50%	traces	traces
t-Bu$_4$CuPc	58%	38%	43%	26%
t-Bu$_4$ZnPc	49%	10%	n /a *	16%

* No formation of the expected product was observed.

Δ= 135 °C (DMAE), 154 °C (anisole (A)),175 °C glycerol/anisole (GA)). Base: 1,8-diazabicyclo(5.4.0)undec-7-ene (DBU), potassium hydroxide (KOH).

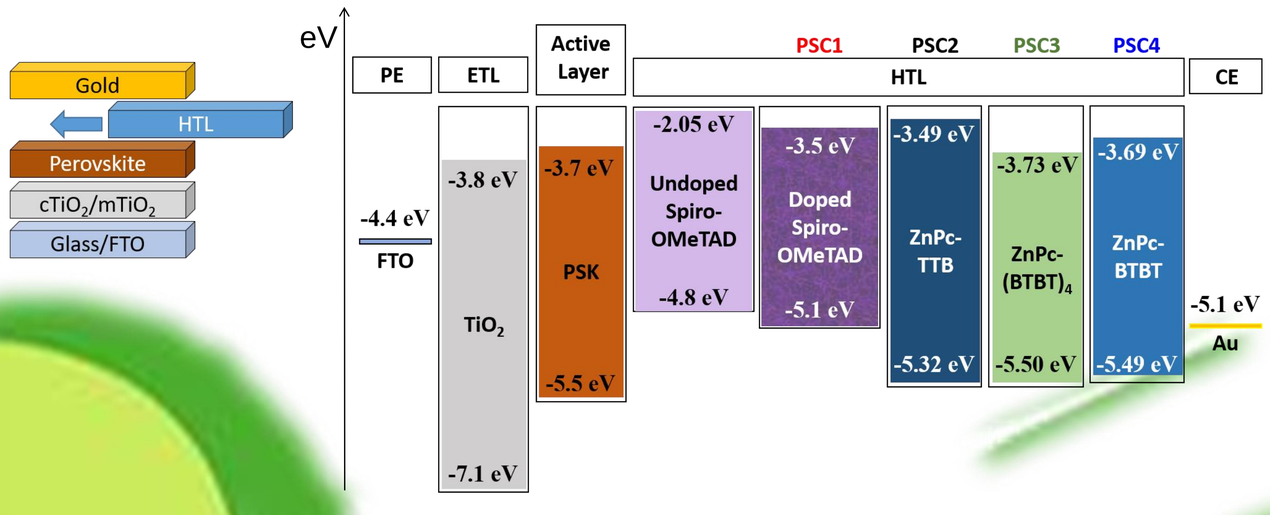




(a) *tert*-butylammonium fluoride trihydrate, $Pd(PPh)_3Cl_2$, THF (only for ZnPc-$(BTBT)_4$), N_2,80°C.

Perovskite solar cells: a topical application target

We report a mesoscopic perovskite solar cell architecture and a schematic representation for the energy band diagram of the materials involved in the tested solar cell structures. In collaboration with CHOSE (Center for Hybrid and Organic Solar Energy).



	V_{oc} [avg.V_{oc}] [V]	J_{SC} [avg.J_{SC}] [mA cm^{-2}]	FF [avg.FF] [%]	PCE [avg.PCE] [%]	R_S [Ω cm^{-2}]
Spiro-OMeTAD	1.05 (1.04)	23.5 (21.9)	77.3 (74.3)	18.7 (16.9)	1.28 (1.52)
UD-ZnPc-TTB	1.02 (1.00)	23.5 (22.5)	67.7 (62.8)	15.4 (14.2)	1.07 (1.49)
D-ZnPc-TTB	1.03 (1.01)	22.8 (22.1)	70.5 (65.1)	16.0 (14.7)	1.01 (1.53)
UD-ZnPc-$(BTBT)_4$	1.01 (1.00)	21.9 (20.7)	66.5 (62.4)	14.0 (13.0)	2.17 (2.08)
D-ZnPc-$(BTBT)_4$	0.99 (0,98)	22.4 (22.2)	65.9 (63.6)	14.4 (13.8)	2.20 (1.27)
UD-ZnPc-BTBT	0.97 (0.92)	21.5 (20.1)	61.5 (55.4)	11.8 (10.3)	3.71 (4.35)
D-ZnPc-BTBT	0.93 (0.88)	19.0 (17.5)	57.2 (53.4)	9.0 (8.3)	5.56 (6.30)

UD = undoped
D = doped (spiro-OMeTAD solution (73.5g/ml) in chlorobenzene (CB) was doped with TBP (26.7ml/ml) and LiTFSI (16.6 ml/ml); ZnPcs solutions (10 mg/ml) were doped adding 4 ml of TBP and 7,5 ml of LiTFSI).

Electrical parameters for the best efficient device for each tested cell structure.

Zanotti, G. et al. ChemPlusChem 2020, 85, 1-12; Zanotti, G. et al. Molecules 2021, 26, 1760.

This work has been financially supported by PRIN2017-BOOSTER (ID: 2017YXX8AZ) and PON «R&I» 2014-2020-BEST4U.