

Orienta Tesi

*Cdl Chimica e
Scienze Chimiche*



chimica_unibas



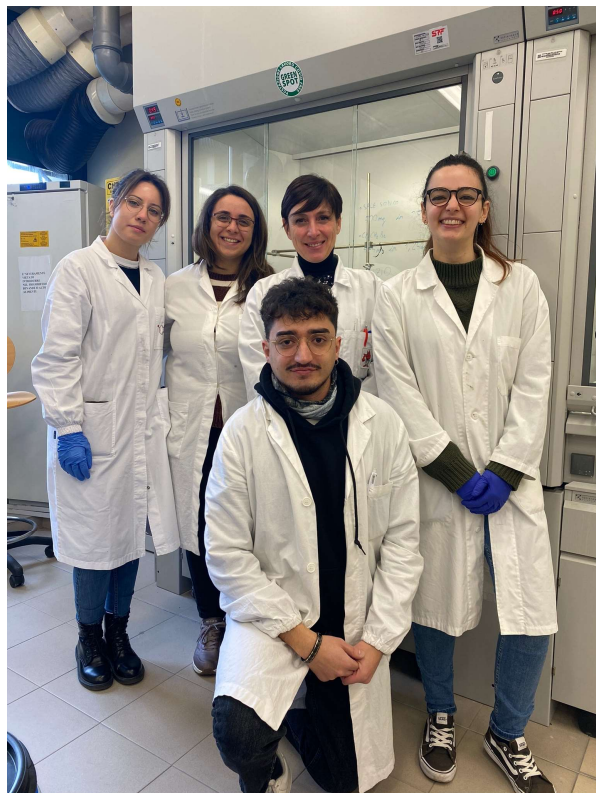
CdL Chimica Unibas

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esperimenti"



Dipartimento di Scienze

LABORATORIO DI CHIMICA INORGANICA



Responsabile Scientifico:
dott.ssa Sandra Belviso



Potenza, 31 gennaio 2023



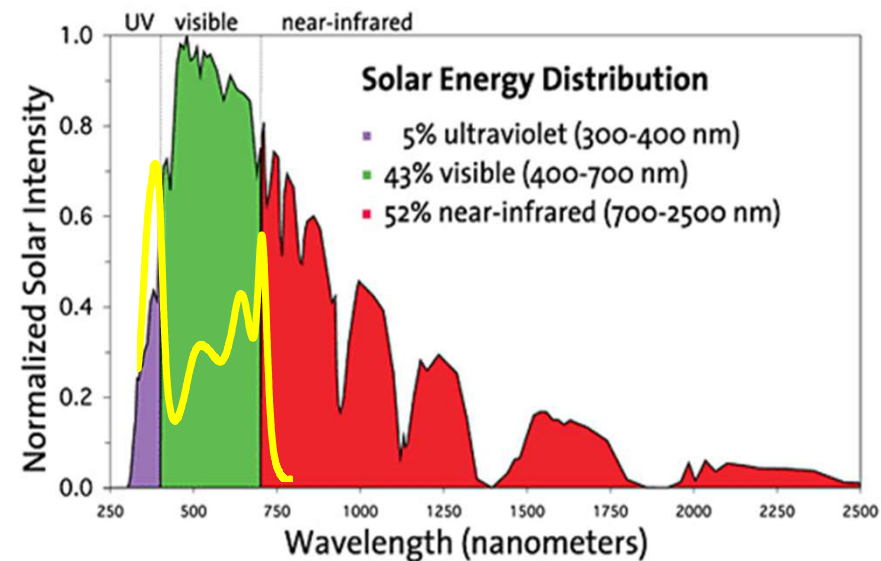
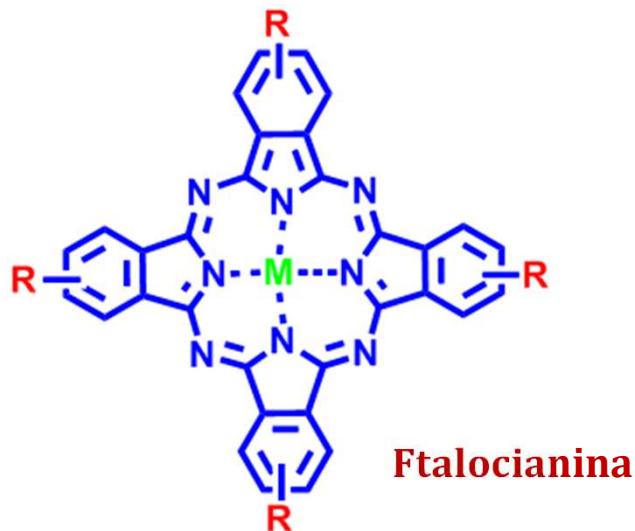
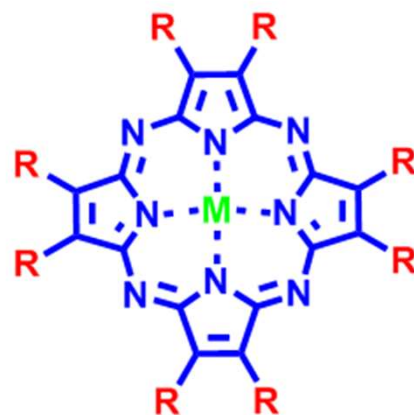
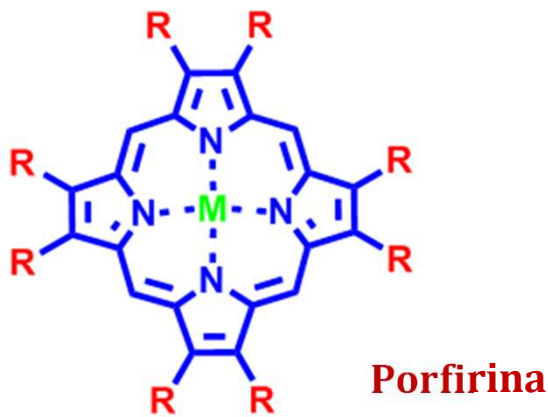
Attività di ricerca

Sintesi e caratterizzazione di **composti di coordinazione** per la realizzazione di **materiali innovativi** da impiegare:

- nei settori dell'optoelettronica
- nel fotovoltaico di nuova generazione (Fotovoltaico Organico)
- in campo ambientale

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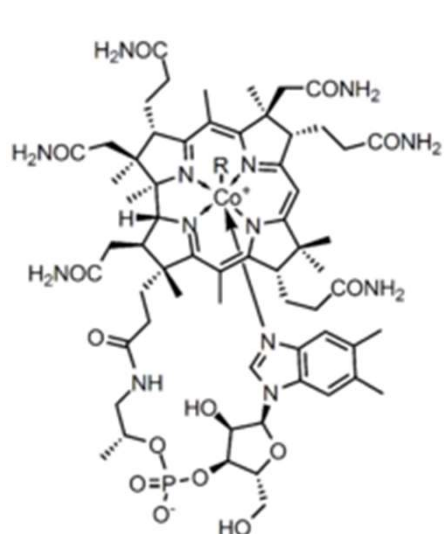
Macro cicli Tetrapirrolici: dalla Natura ai nuovi materiali



- Assorbimento che copre bene l'emissione solare nel visibile
- Facile modulabilità strutturale

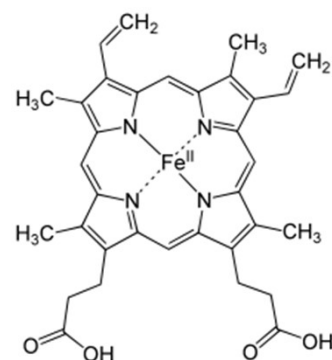
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Macroцици tetrapirrolici di importanza biologica

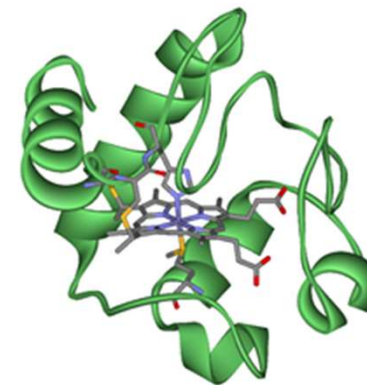


Vitamina B12

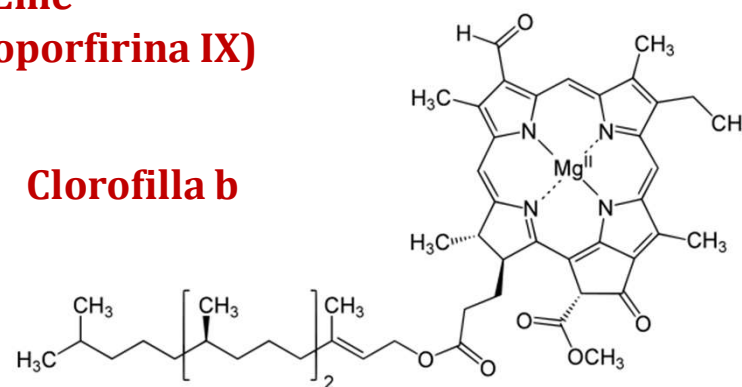
R = 5'-deoxyadenosyl, Me, OH, CN



**Eme
(Fe-Protoporfirina IX)**



Citocromo C



Clorofilla b

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Macroцици tetrapirrolici nella scienza dei materiali

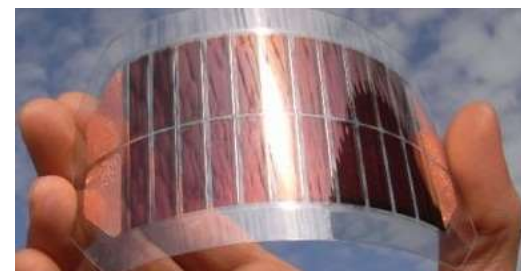
- **Cristalli Liquidi (LC)**



- **Ottica non lineare (NLO)**

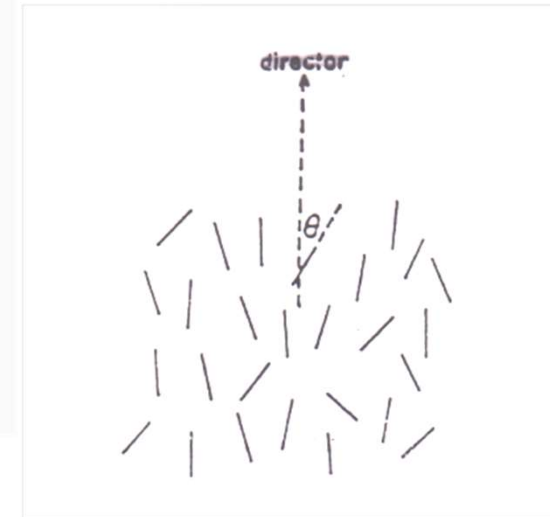
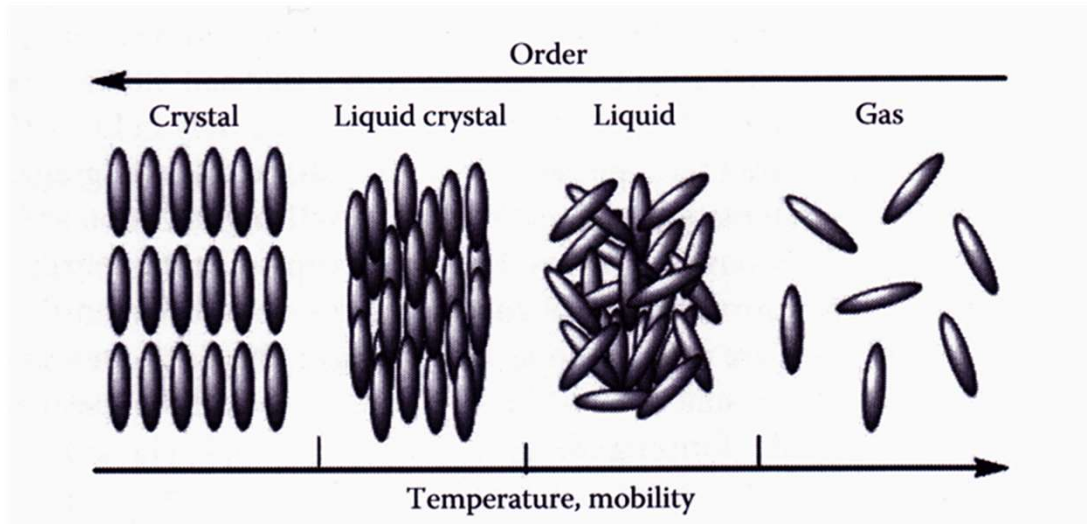


- **Fotovoltaico Organico (OPV)**



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Stato Liquido-Cristallino (fase mesomorfa)

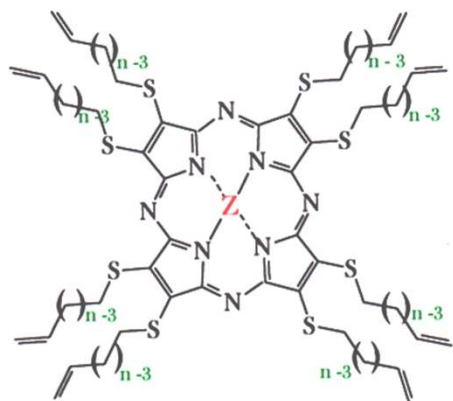


Parziale ordine **posizionale** ed **orientazionale**



ANISOTROPIA E FLUIDITA'

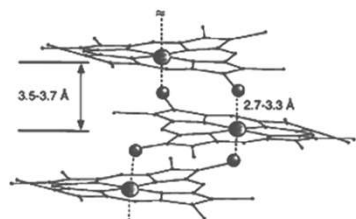
Tioalchil porfirazine: fasi Liquido-Cristalline stabili e di tipo colonnare



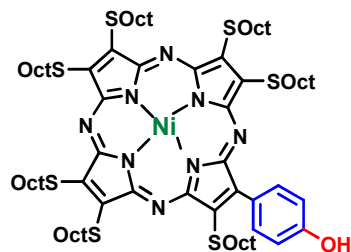
Z = Co, Ni, Cu, H₂

n = 4, 5, 6, 8

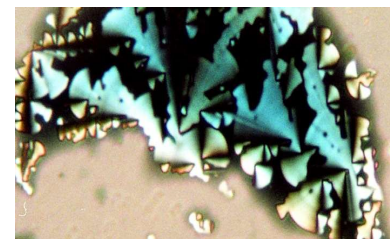
[Z(oaspz)]



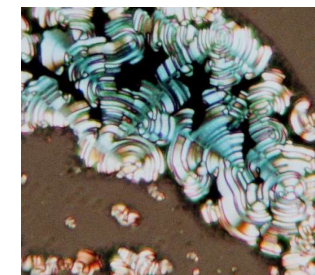
\mathcal{D}_h



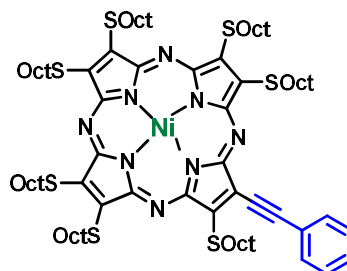
$\Delta T = 63.0^\circ\text{C}$



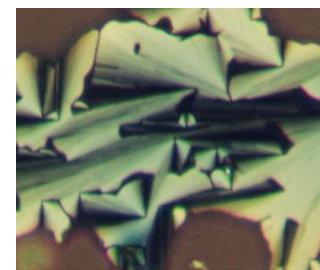
T = 83.1°C



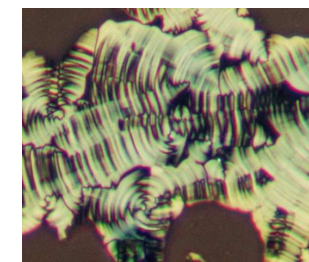
T = 63.4°C



$\Delta T = 73.8^\circ\text{C}$



T = 110.0°C



T = 25.0°C



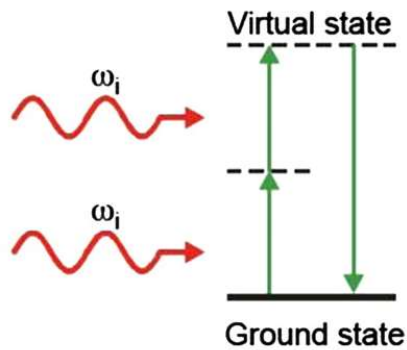
S. Belviso et al., *J. Mater. Chem.* **2000**, 10, 297.

S. Belviso et al., *Dalton Trans.*, **2015**, 44, 2191.

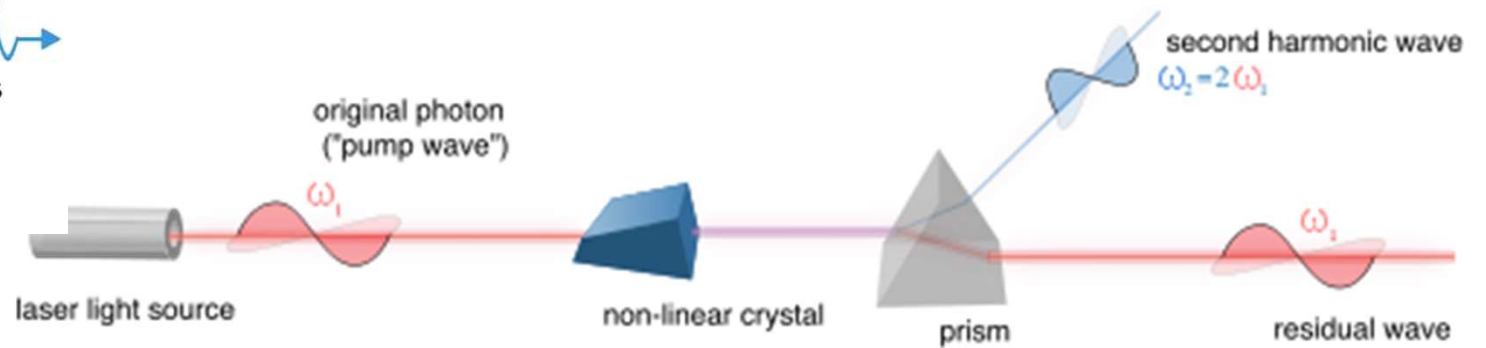
S. Belviso et al., *J. Porphyrins Phthalocyanines*, **2016**, 20, 223.

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Ottica Non Lineare del Secondo Ordine



Generazione di seconda armonica(SHG)



Conversione della luce **rossa (1064 nm)** del laser in **luce verde(532 nm)**

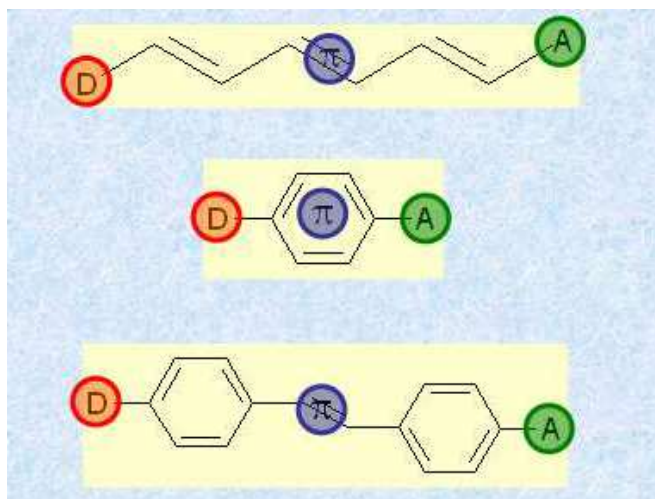
Blu-ray laser



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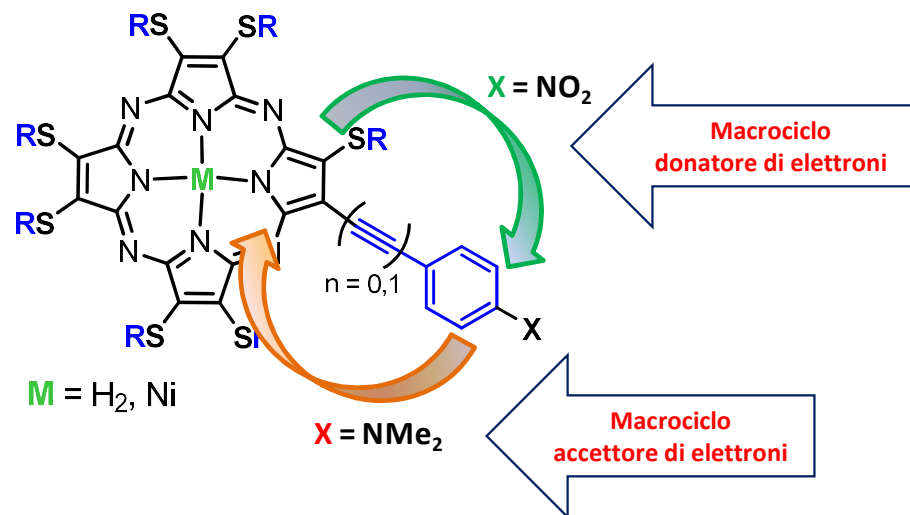
NLO: sistemi molecolari "Push-Pull" porfirazinicci

Struttura generale di sistemi "Push-Pull"



D = elettron-donatore
A = elettron-accettore

Tioalchil Porfirazine: Sistemi "Push-pull" **non** convenzionali



Composto	$\mu(D)$ (CH_2Cl_2)	$\mu\beta_{1907}^a$ ($\times 10^{-48}$ esu)
NO_2	7.9165	720 @ $5 \times 10^{-4} M$
NMe_2	14.9817	842 @ $5 \times 10^{-4} M$

Tecnologie Fotovoltaiche



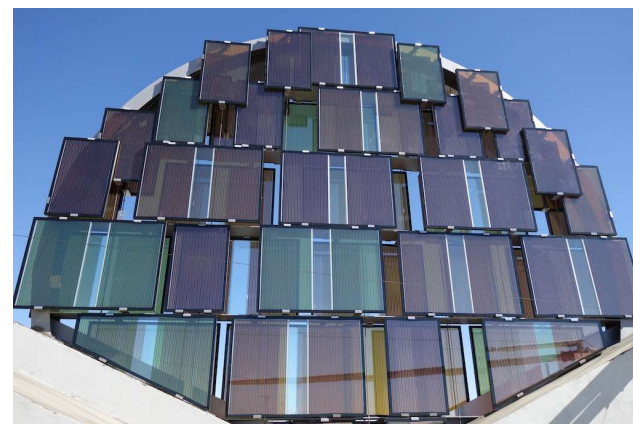
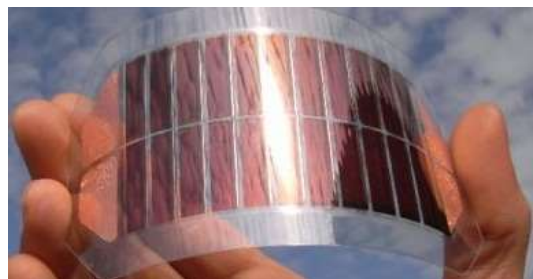
Celle Inorganiche (silicio)

- Efficienza alta
- Stabilità
- Costi alti
- Processo di produzione complesso
- Celle rigide e non trasparenti



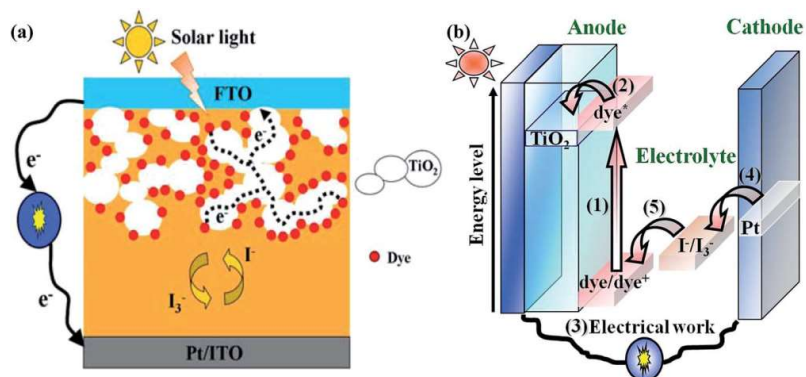
Celle Organiche (molecolari)

- Bassi costi di produzione
- Produzione a stampa ink-jet
- Pannelli leggeri, flessibili, grandi e trasparenti
- Integrazione architettonica
- Modulabilità delle proprietà
- Efficienza inferiore



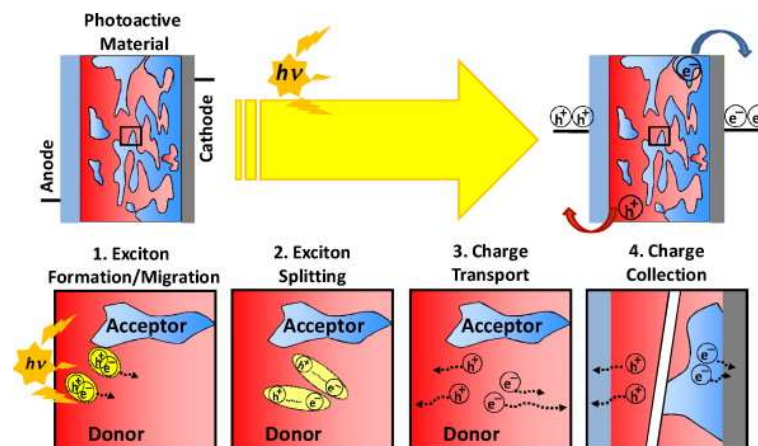
Tipi di Celle solari per OPV

DSSC (dye-sensitized solar cell)



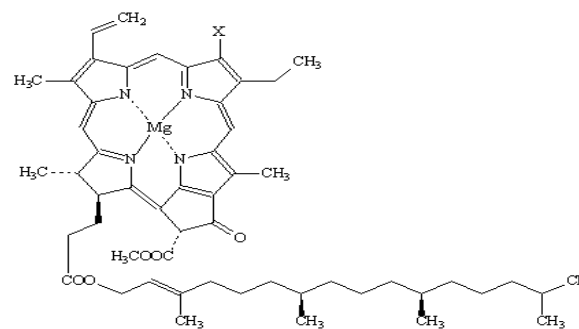
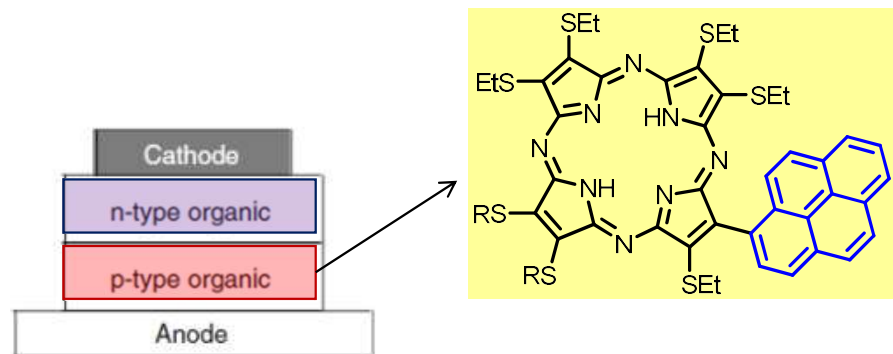
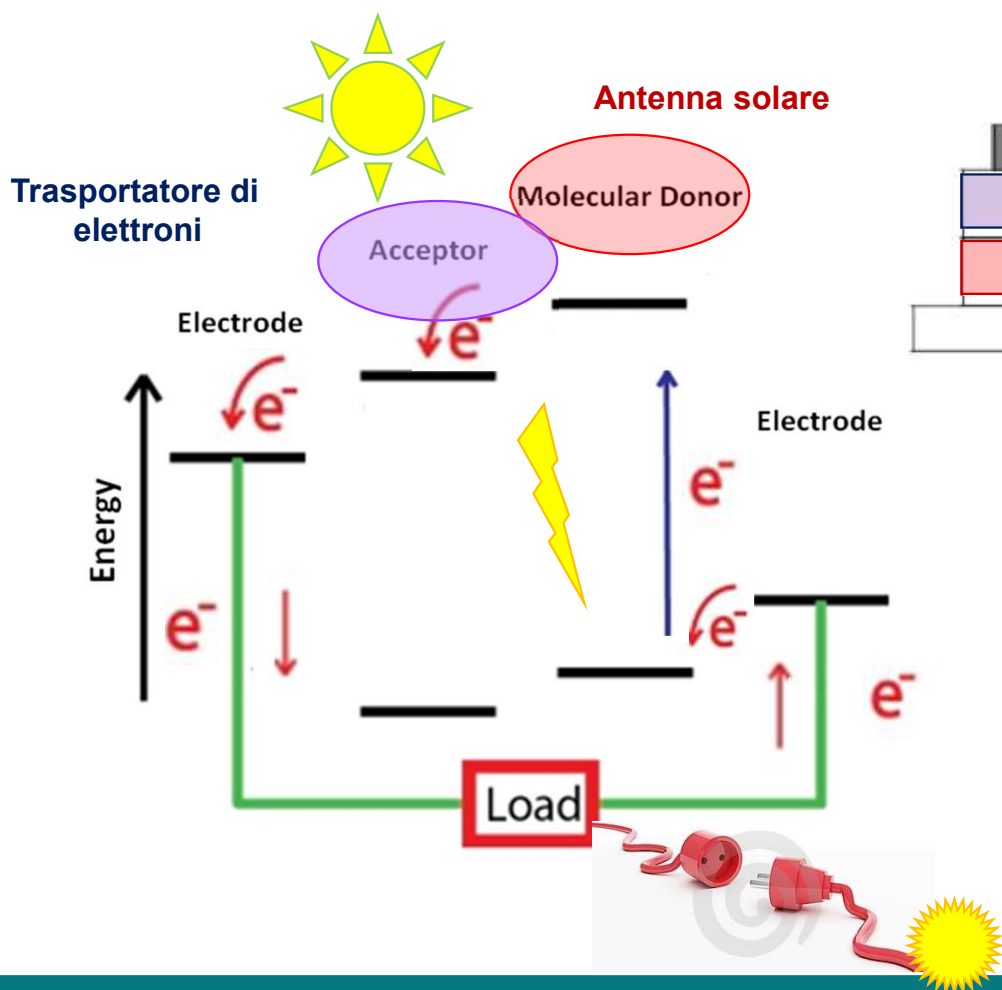
- Unità assorbente ancorata ad un semiconduttore (TiO_2) che funge da accettore di elettroni
- TiO_2 depositato su un elettrodo trasparente che fa passare la luce
- L'elettrone viaggia verso il controelettrodo e viene poi ripristinato al dye attraverso la coppia redox I^-/I_3^-

BHJ (bulk heterojunction)

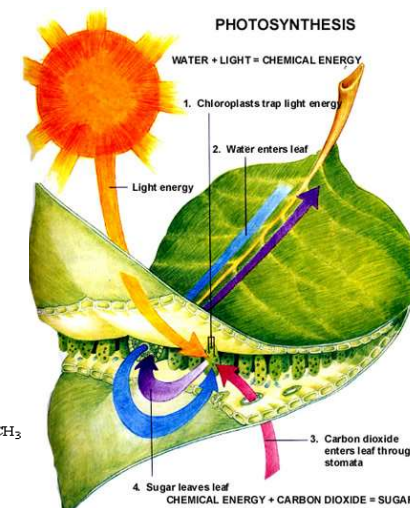


- Vengono mescolati due composti organici che fungono da donatore e accettore di elettroni
- Il composto ottenuto viene racchiuso tra due elettrodi
- Si formano gli eccitoni che devono essere efficacemente separati all'interfaccia tra i due componenti
- Gli elettroni e le buche migrano in direzione opposta generando corrente

Funzionamento delle celle fotovoltaiche organiche



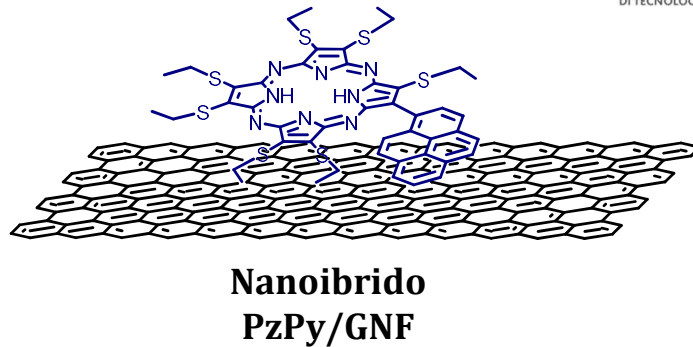
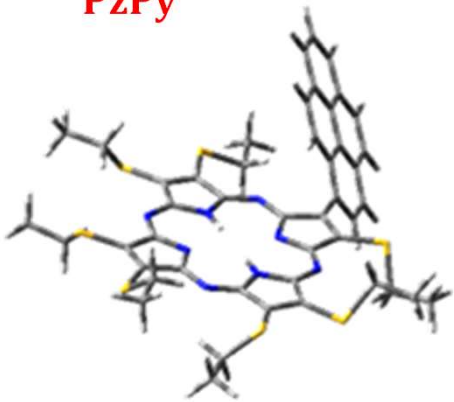
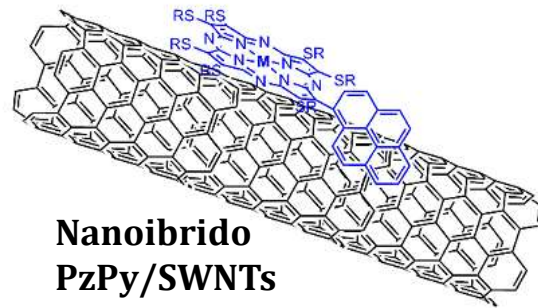
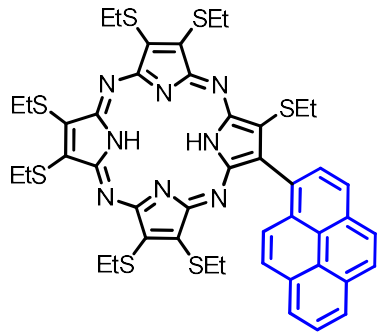
Clorofilla: un'antenna solare



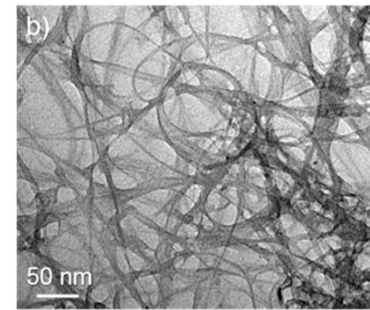
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Tioalchil Porfirazine per Celle OPV di tipo BHJ

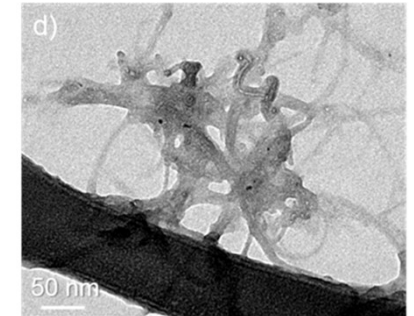
Nanoibridi formati da porfirazine (DONATORI) con nanostrutture di carbonio (ACCETTORI)



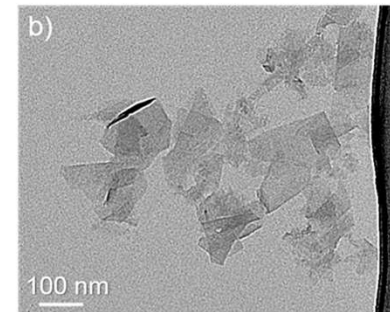
Microscopia elettronica TEM



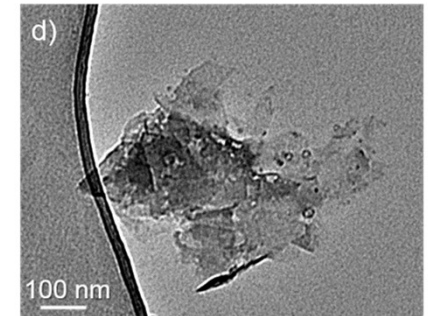
Nanotubi (SWNTs)



**Nanoibridi
PzPy/SWNTs**



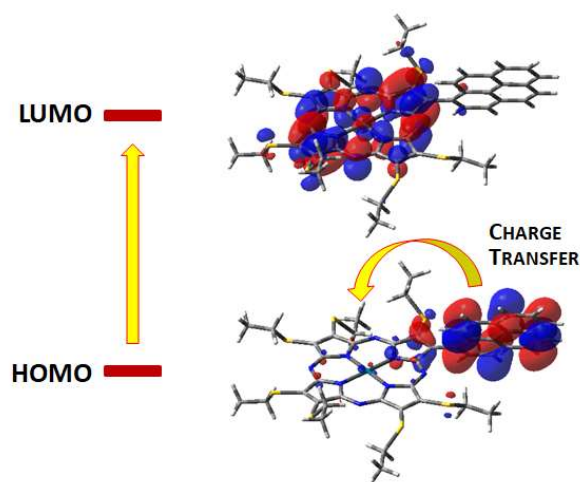
**Nanoflocchi di
grafene (GNF)**



**Nanoibridi
PzPy/GNF**

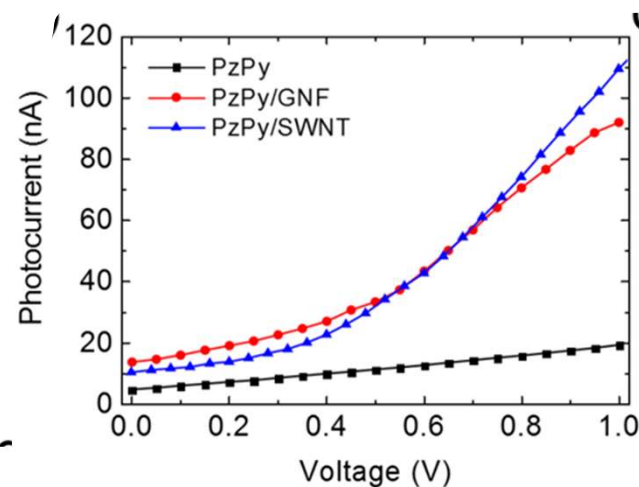
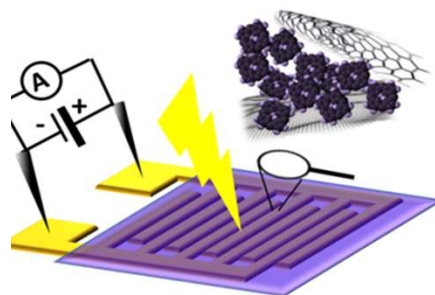
Tioalchil Porfirazine per Celle OPV di tipo BHJ

FOTOGENERAZIONE DI CORRENTE da parte dei nanoibridi PzPy/SWNTs e PzPy/GNF



TD-DFT

NLO



Focorrente generata con irradiazione a 500 nm

Tioalchil Porfirazine per Celle OPV di tipo DSSC



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DI MILANO

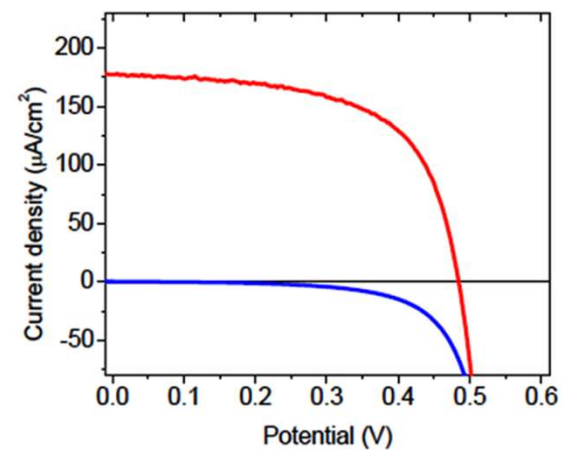
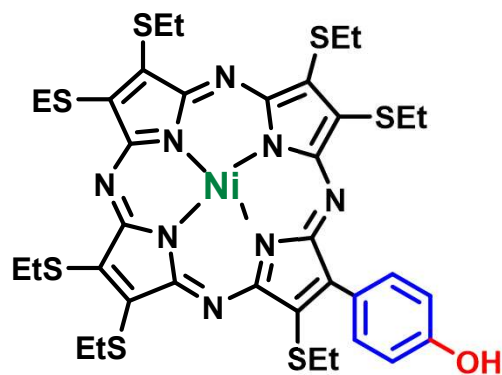
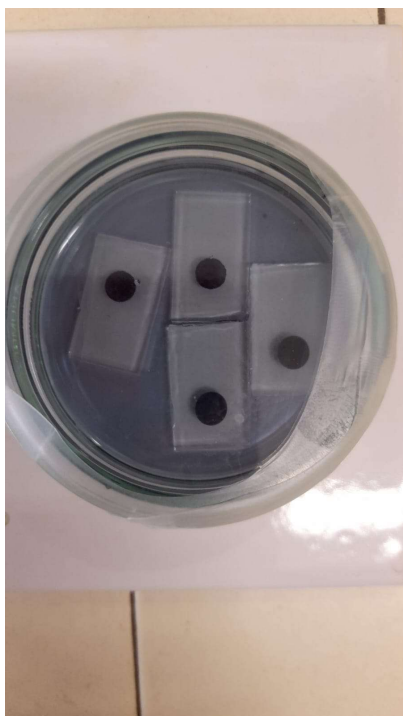
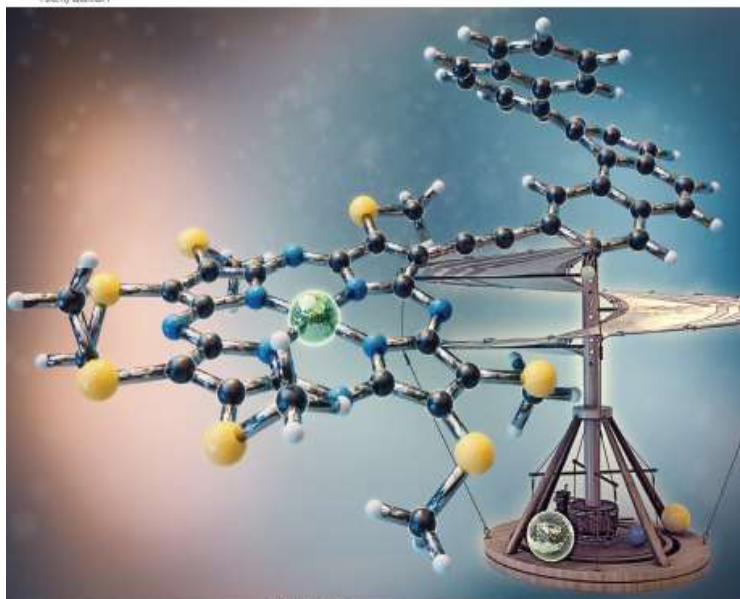


Figure S21. JV characteristics of TiO₂-DSSC with dye 2 under simulated one sun illumination (AM1.5G, P_{in} = 100 mW/cm²) and active area of 0.159 cm².

Dalton Transactions

An international journal of inorganic chemistry
rsc.li/dalton

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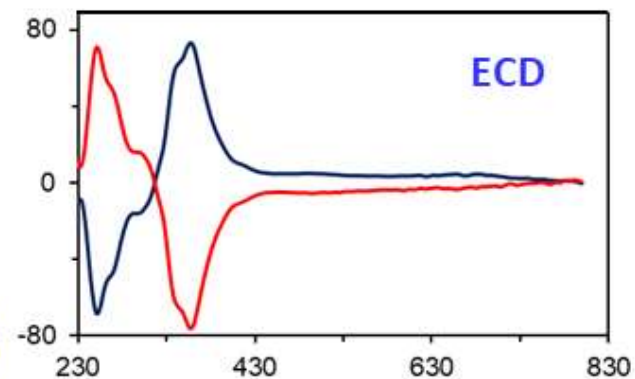
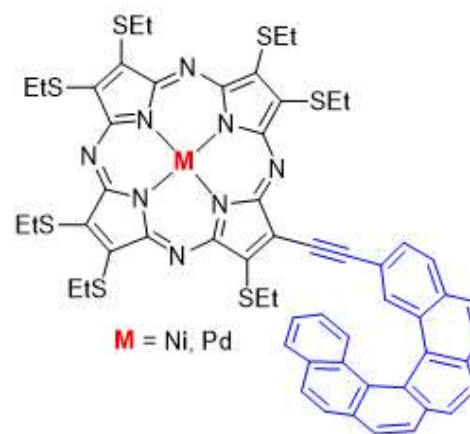


ISSN 1477-922E

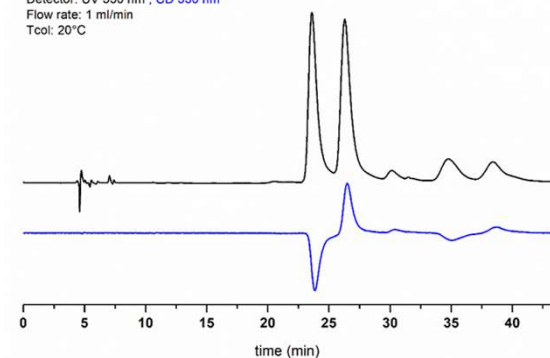


PAPER
Sandra Belviso, Giovanna Longhi et al.
Inherently chiral helicene-substituted thiazolyl porphyrazine
complexes: synthesis and electronic and chiroptical
properties

Tioalchil porfirazine Chirali per OPV



NIPzHelix
Column: (R,R)-Wheik01 400mm*4.6 mm (L*1.D.) 5µm particle size
Eluent: Hex/CH₂Cl₂ 75/25 + 5%EtOH
Detector: UV 330 nm ; CD 330 nm
Flow rate: 1 ml/min
Tcol: 20°C



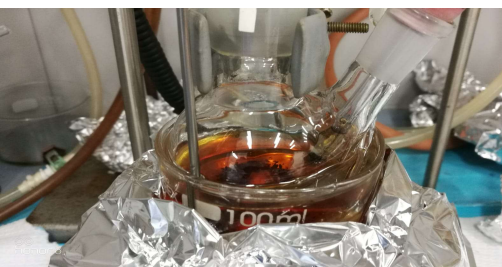
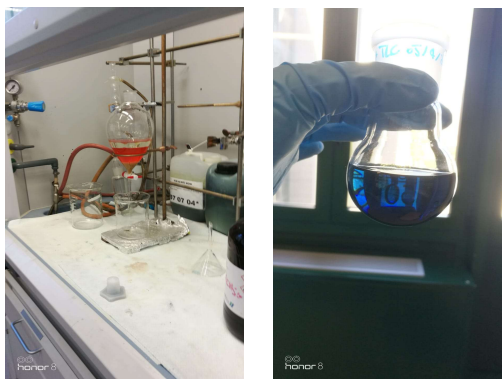
S. Belviso *et al.*, *Dalton Trans.*, 2022, 51, 16453.

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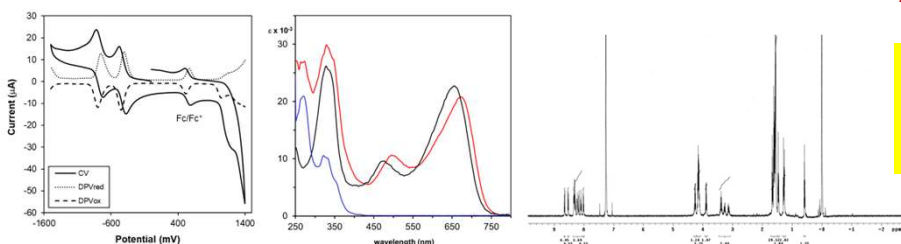
Argomenti per la Tesi di Laurea



- **Sintesi**, caratterizzazione, studio della reattività di **macrocicli tetrapirrolici** e loro complessi metallici
- Preparazione di materiali tetrapirrolici innovativi per **celle fotovoltaiche organiche** di tipo DSSC e BHJ
- Studio dei fenomeni di **aggregazione** di macrocicli tetrapirrolici per interazioni con **nanotubi** e **grafene** e per riconoscimento chirale

**Piano Nazionale di Ripresa e Resilienza (PNRR)
Ecosistema Tech4You - Spoke 2 G02.1 PP1 - Azione 1**

Titolo del Progetto: *Materiali innovativi per la produzione di energia da fonte solare*



Potenza, 31 gennaio 2023