

Computational discovery, design and optimisation of organic molecules for application in optoelectronic devices



UNIVERSITÀ
DI SIENA
1240

**Prof. Daniele
Padula**

**Dipartimento di
Biotecnologie,
Chimica e
Farmacia
Università di
Siena**

Research activity

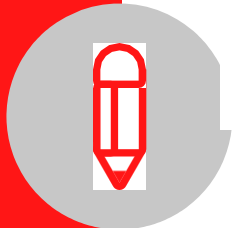


Our research focuses on the computational discovery and design of new organic materials for application in optoelectronic devices used in clean energy production and with low energy consumption (photovoltaic devices, OLEDs, OFETs), with efforts in the understanding and characterisation of fundamental photophysical processes occurring in such devices.

In this field, we exploit a wide set of computational methods, ranging from quantum mechanics, to classical physics, also including Machine Learning algorithms.

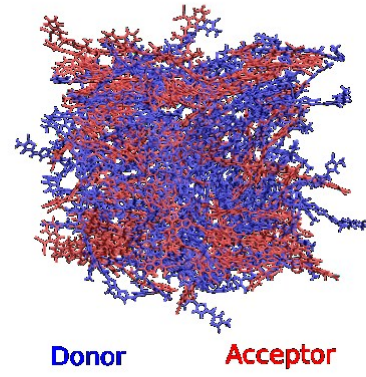
Furthermore, we realise computational studies on organic reaction mechanisms of industrial interest in the production of important synthetic intermediates, or for the release of small molecules (drugs) under mild conditions.

Images

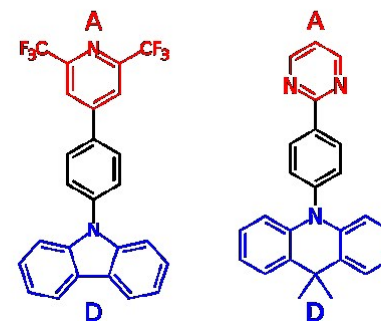


Organic Photovoltaics

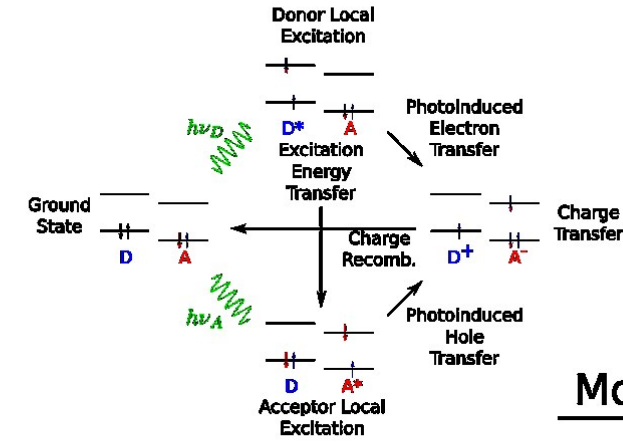
Classical MD
FF parameterisation



OLEDs

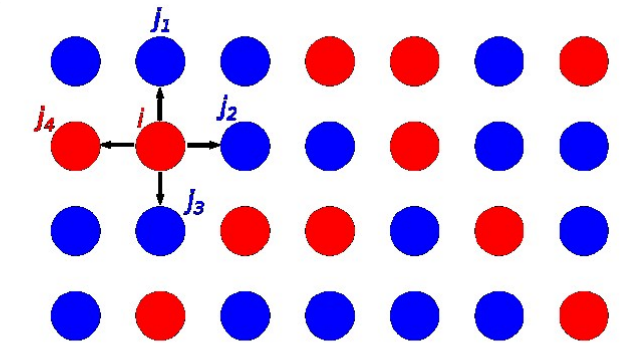
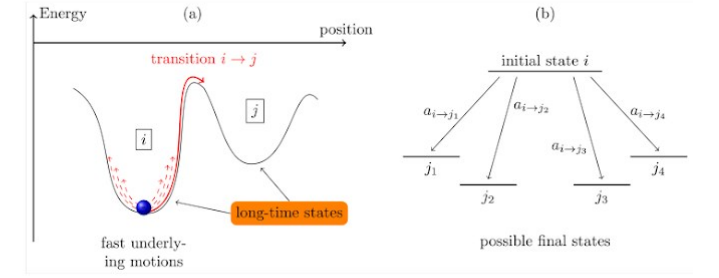


Electronic Modelling
of Fundamental Processes

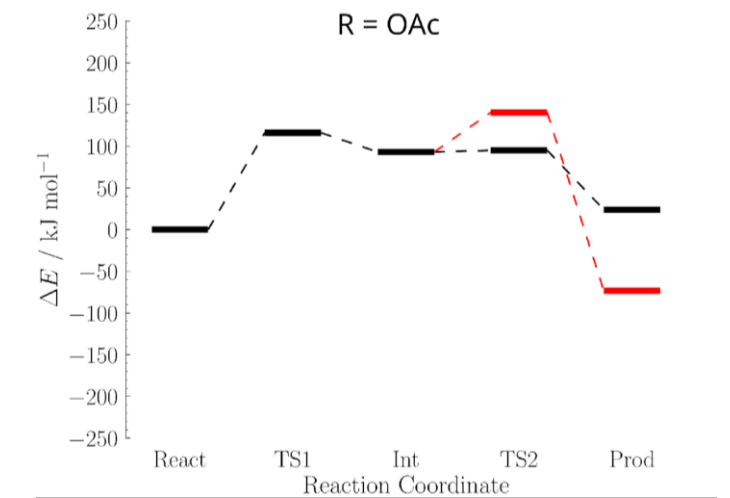


Morphology
Rates

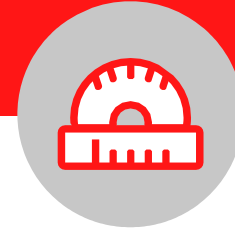
Model Reduction



Reaction mechanisms for the release of small molecules (drugs).



Technologies and services



We exploit a High-Performance Computing infrastructure available in our Department, and national computational resources accessible upon request (CINECA). Services for companies involve theoretical studies for the understanding of a specific process (chemical reaction or device operational detail), finalised at its improvement in terms of efficiency.

Applications and collaborations



We have collaborated with an Italian pharmaceutical company (Recipharm) on the detailed mechanistic study for an industrial process. We have also collaborated with foreign companies interested in the development of new luminescent organic materials for displays of electronic devices.

Finally, we have an on-going collaboration with Lavazza and ICCOM-CNR (Pisa) for the development of recyclable coffee capsules made of organic polymers.

For more information



Tech Transfer Office of University of Siena

Headquarters: Banchi di sotto,55 - Siena

Web site: <http://research.unisi.it>

E-mail: ricerca@unisi.it - liaison@unisi.it

For more information



Ufficio Regionale di Trasferimento Tecnologico

Headquarters: Via Luigi Carlo Farini, 8 - 50121 Firenze, FI

E-mail: urtt@regione.toscana.it