SCIENZE E TECNOLOGIE CHIMICHE

TESI DI LAUREA TRIENNALE E DI LAUREA MAGISTRALE PRESSO IL NANOQLAB

Prof. CRISTIANA DI VALENTIN

DIPARTIMENTO DI SCIENZA DEI MATERIALI
CENTRO DI BIONANOMEDICINA
UNIVERSITÀ DI MILANO-BICOCCA

www.nanoQlab.mater.unimib.it

MILANO 21/10/2022

IL GRUPPO

MILANO 21/10/2022

IL LABORATORIO

QUESTO È L'UFFICIO DEI NOSTRI SOGNI!

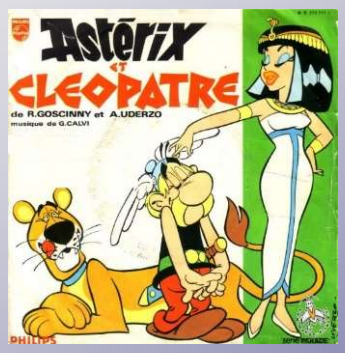
MILANO 21/10/2022

STRUMENTAZIONE DI CALCOLO AD ALTE PRESTAZIONI

LABORATORIO
DI CHIMICA QUANTISTICA
PER LA NANOMEDICINA

COORDINATO DA: CRISTIANA DI VALENTIN
HPC SPECIALIST: LORENZO FERRARO

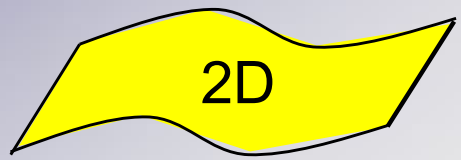
X86/CPUs ARCHITECTURE
60 TFLOPS
1500 cores
Xeon processors 2.6 GHz
7.5 TB RAM
Infiniband 56 Gbit/s
STORAGE 150 TB RAW
Integrated cooling systems



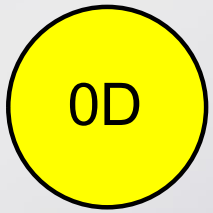
CENTRO DI NANOMEDICINA
MILANO BICOCCA
MONZA

MILANO 21/10/2022

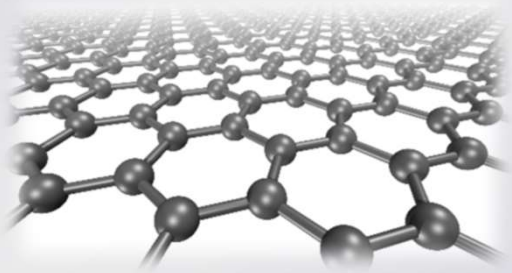
STUDI DI CHIMICA COMPUTAZIONALE DI MATERIALI NANODIMENSIONATI E NANOSTRUTTURATI

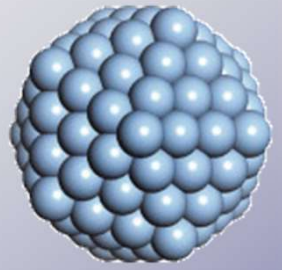


MATERIALI BIDIMENSIONALI
G - GO - hBN - WSe_2 - C_3N_4



NANOPARTICELLE





ALMENO UNA DIMENSIONE NELLA SCALA NANOMETRICA

PER MEDICINA – ENERGIA – AMBIENTE

nanoQlab

Quantum Mechanical Methods

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(\mathrm{r}) + V(r)\Psi(\mathrm{r}) = E\Psi(\mathrm{r})$$

Kinetic Energy + *Potential Energy* = *Total Energy*

but accurate

CRYSTAL — a computational tool for solid state chemistry and physics

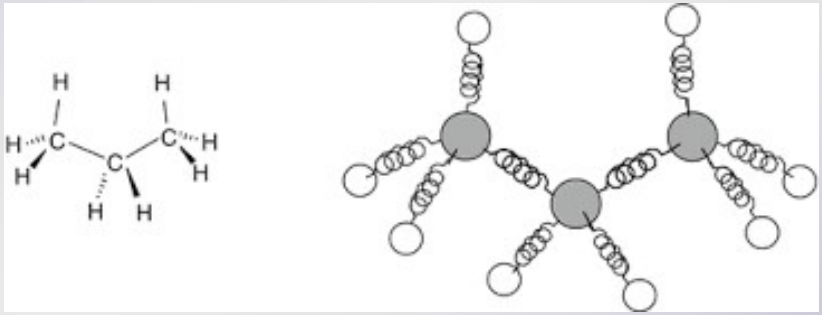
QUANTUM ESPRESSO

Gaussian 16

DFTB

OCTUPUS

Molecular Mechanics Methods



but less accurate

Amber 2018 Reference Manual
(Covers Amber18 and AmberTools18)

GROMACS
FAST. FLEXIBLE. FREE.

NAMD
Scalable Molecular Dynamics

nanoQlab

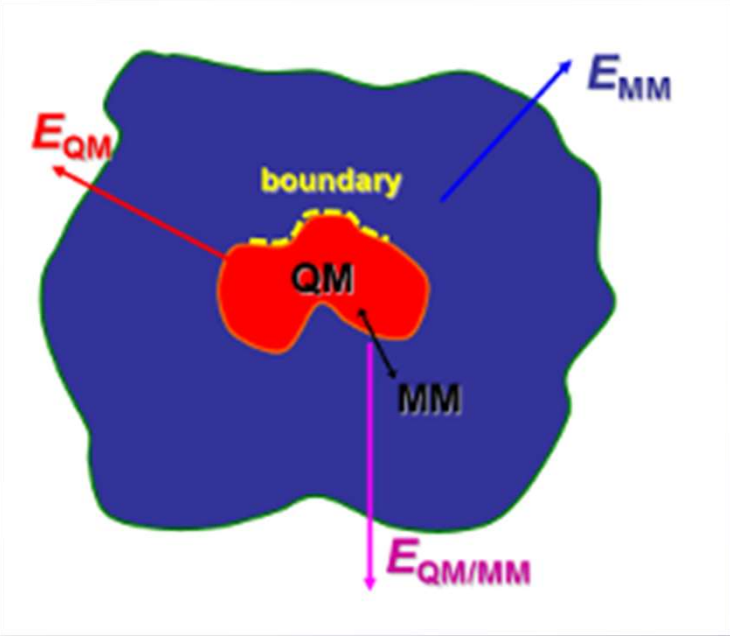
Quantum Mechanical Methods + Molecular Mechanics Methods

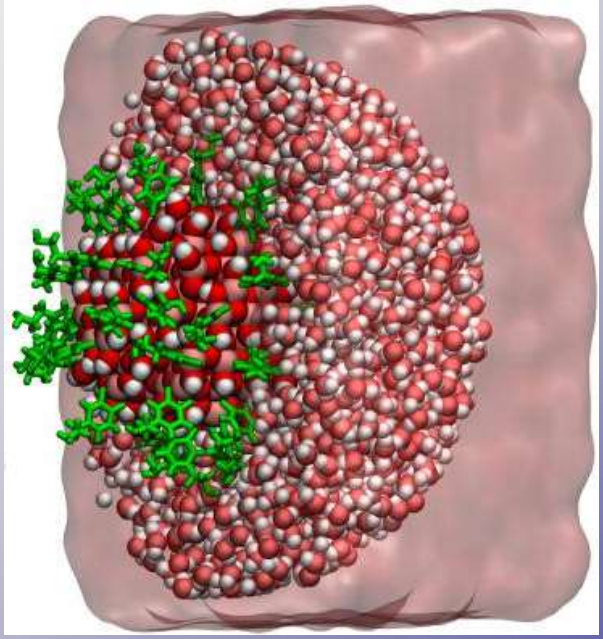
a computational tool for solid state chemistry and physics
CRYSTAL

QM / MM

Amber 2018 Reference Manual
(Covers Amber18 and AmberTools18)

DFTB





Dohn, Selli, Fazio, Ferraro, Mortensen, Civalleri, CDV *Molecule* **2018** 23 2958

Siani, Motta, Ferraro, Dohn, CDV *JCTC.* **2020** 16 6560

NANOMEDICINA BIOINORGANICA

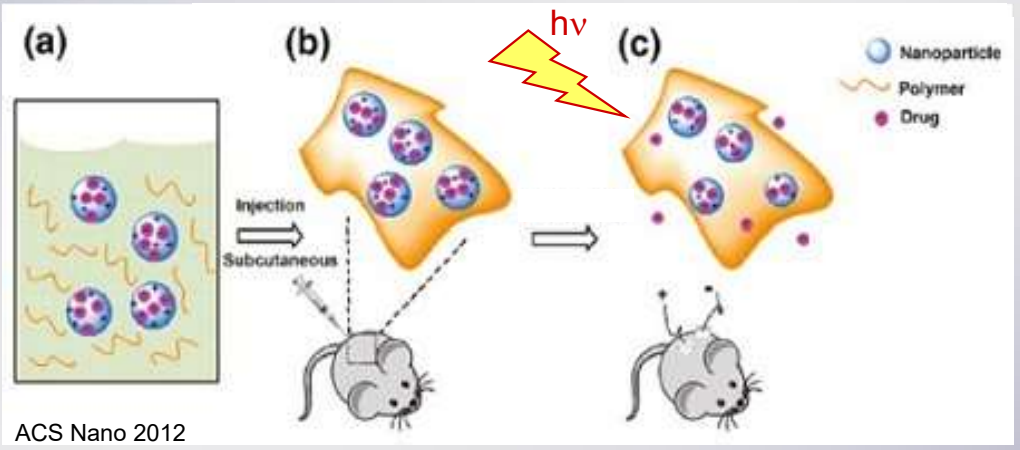
INORGANIC NP + BIOLOGICALLY ACTIVE MOLECULES = NP

BIOMIMESIS – TARGETING – DRUG DELIVERY – THERAPEUTICS – IMAGING

- METAL
- METAL OXIDE
- G or GO FLAKES

TiO_2

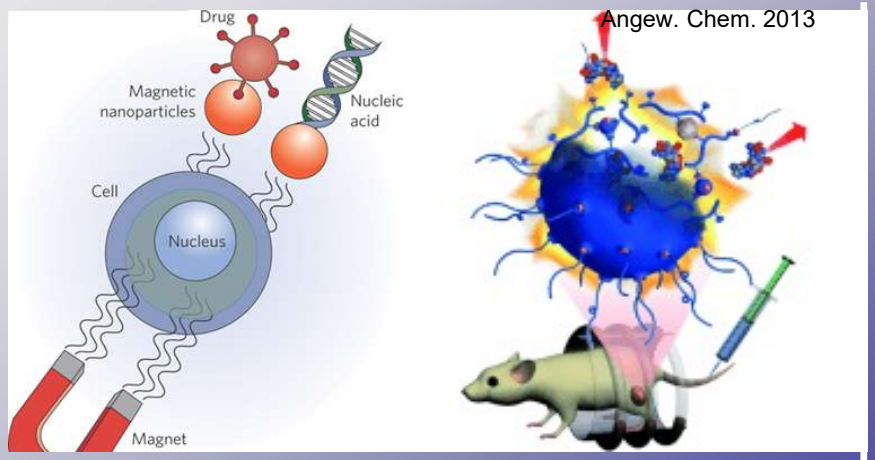
TERAPIA FOTODINAMICA (TiO_2)



ACS Nano 2012

Fe_3O_4

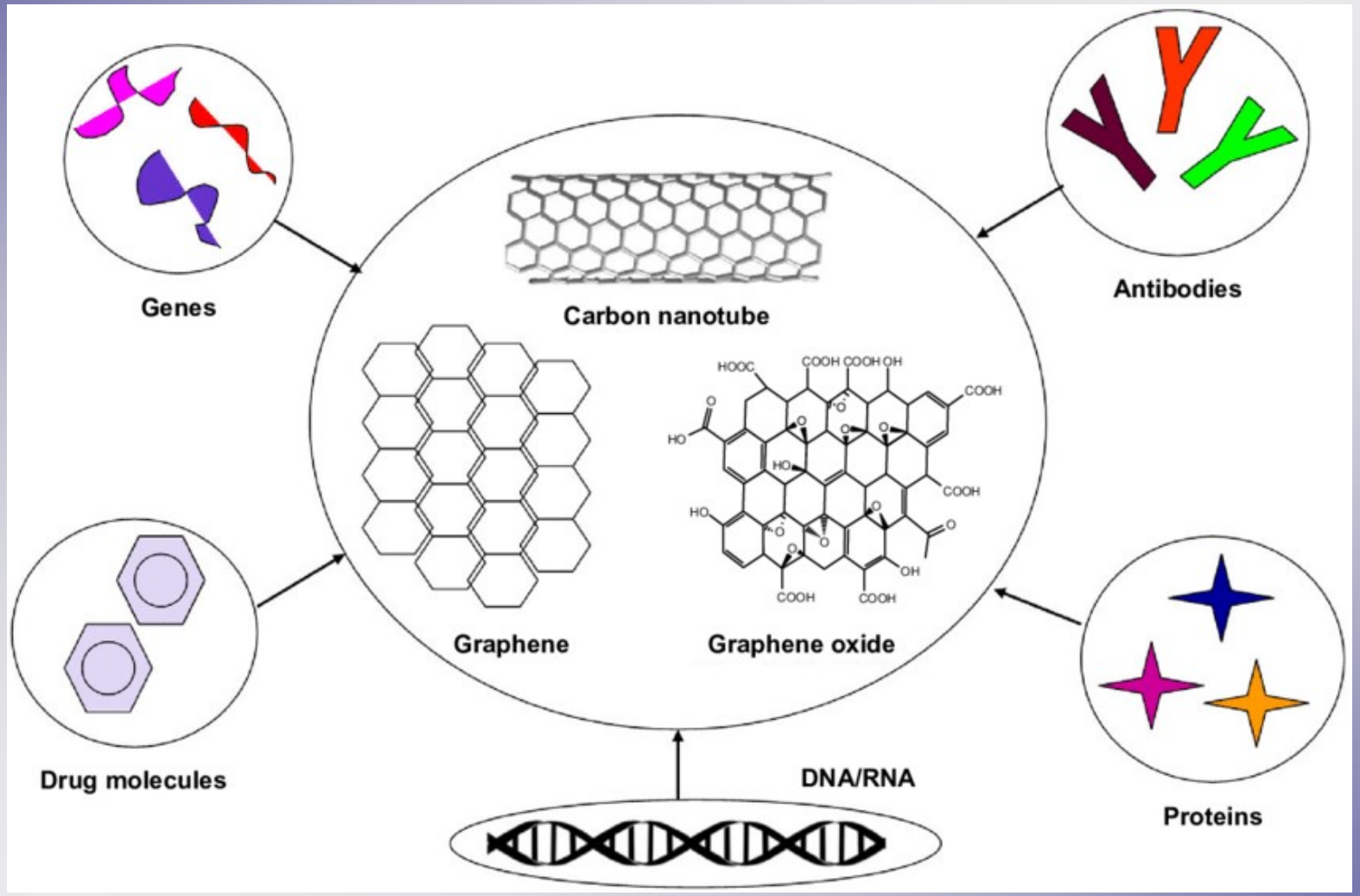
MAGNETISMO (OSSIDI DI FERRO)



SMART STIMULI-RESPONSIVE NANODEVICES

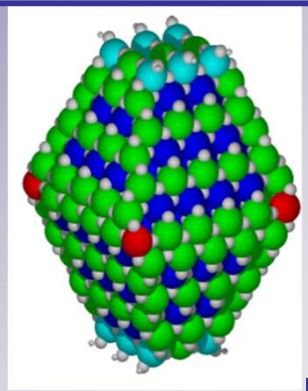
MILANO 21/10/2022

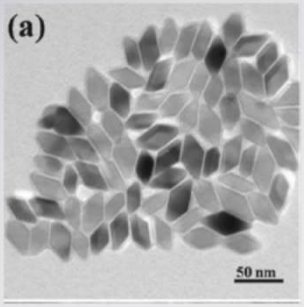
VETTORI PER TRASPORTO



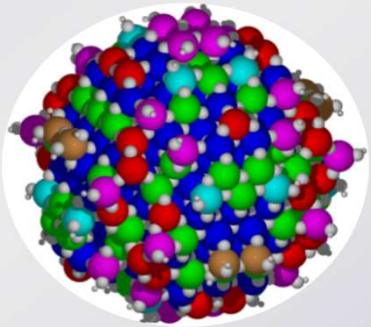
FORMA DELLE NANOPARTICELLE

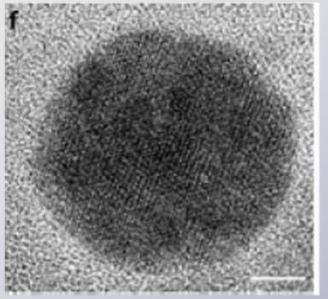
NANOPARTICELLE DI TiO_2





FACETED





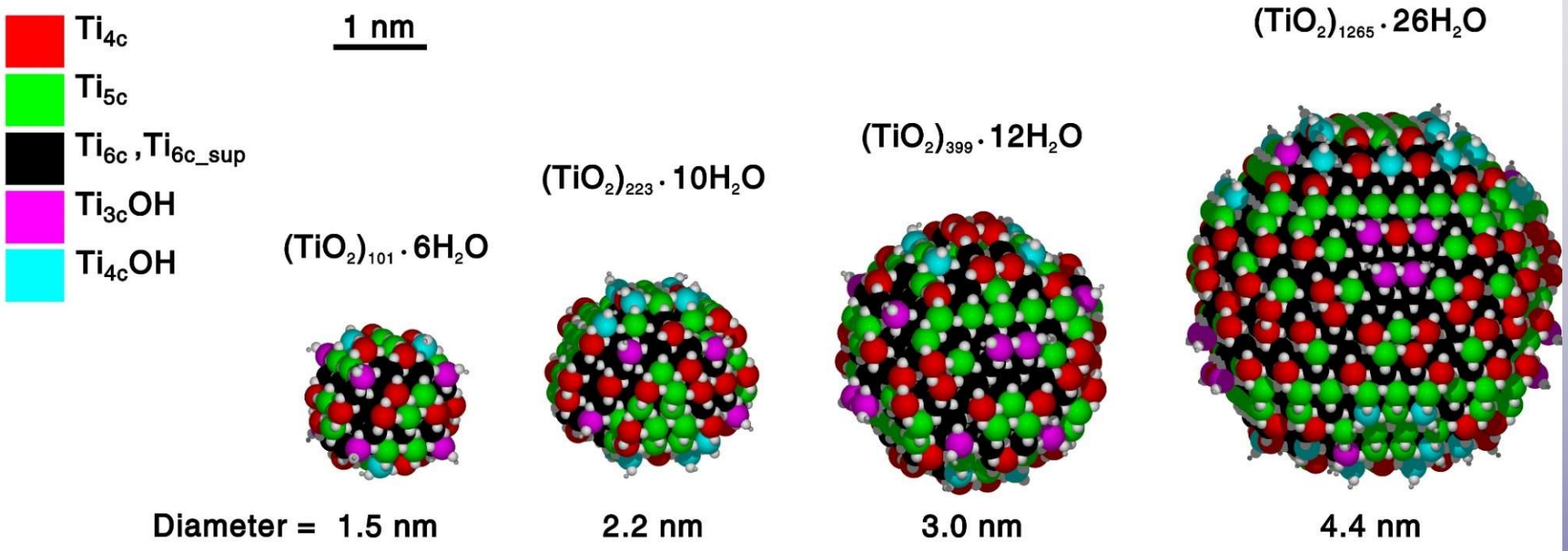
SPHERICAL

WULFF SHAPE PREDICTION:
DECAHEDRON
by Barnard et al. Nano Lett. 2005

LOW PARTICLE DENSITY

Fazio, Ferrighi, CDV*JPC C* 2015 119 20735

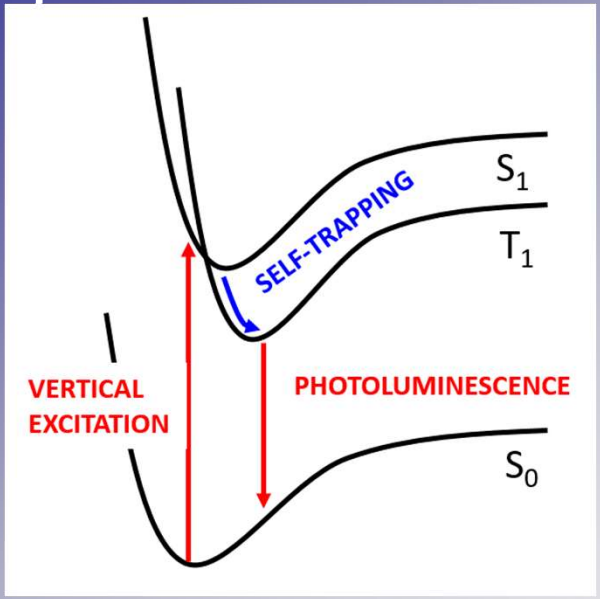
DIMENSIONE DELLE NANOPARTICELLE

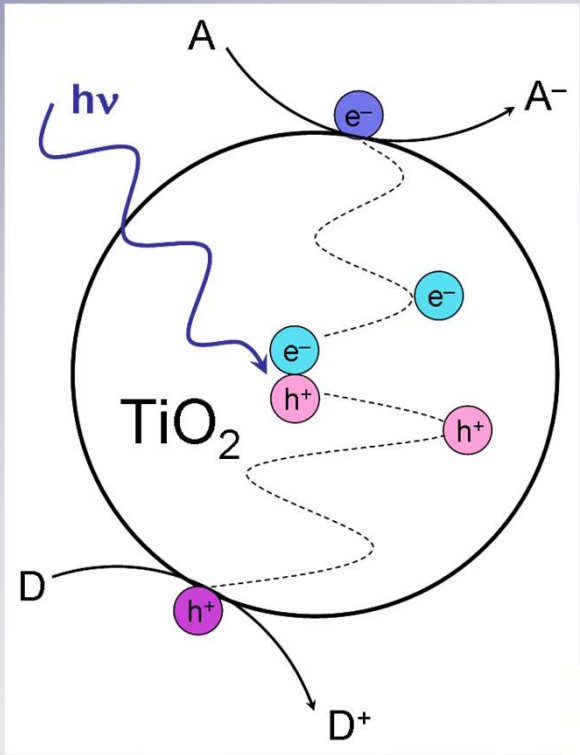


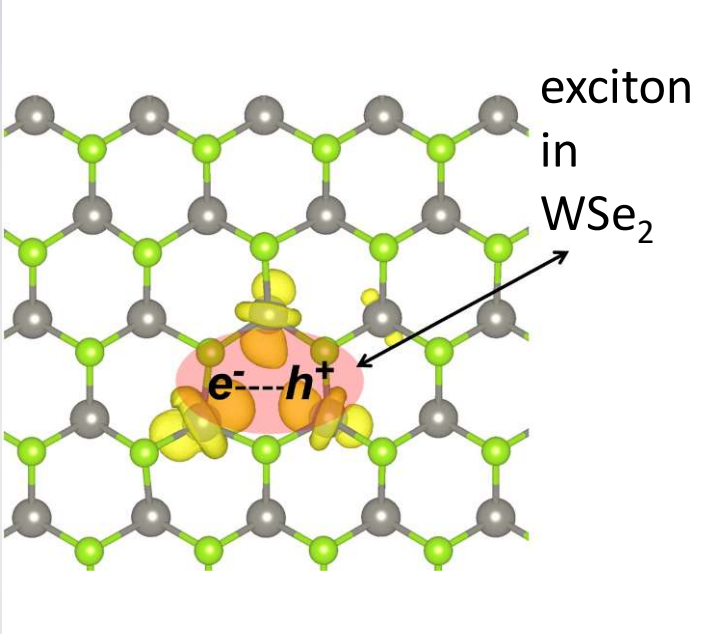
n° of atoms =	321	699	1233	3873

Fazio, Selli, CDV *JCP* **2017** 147 164701

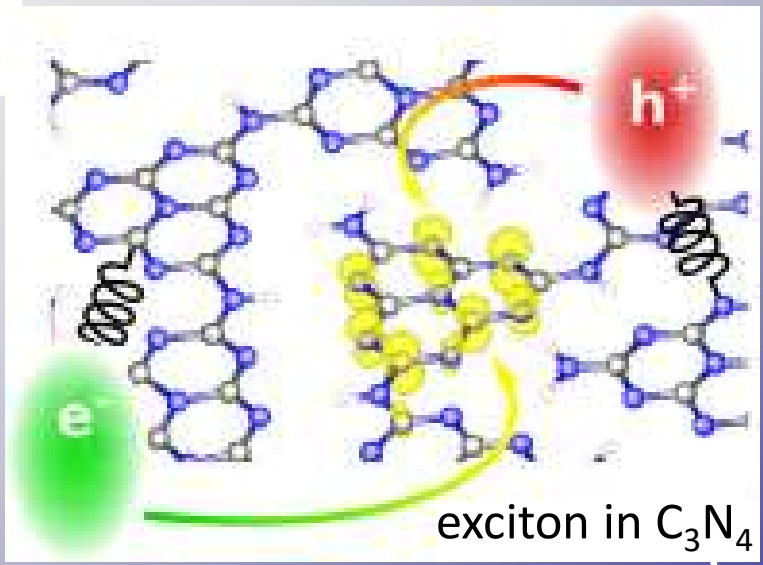
FOTOATTIVAZIONE E STATI ECCITATI





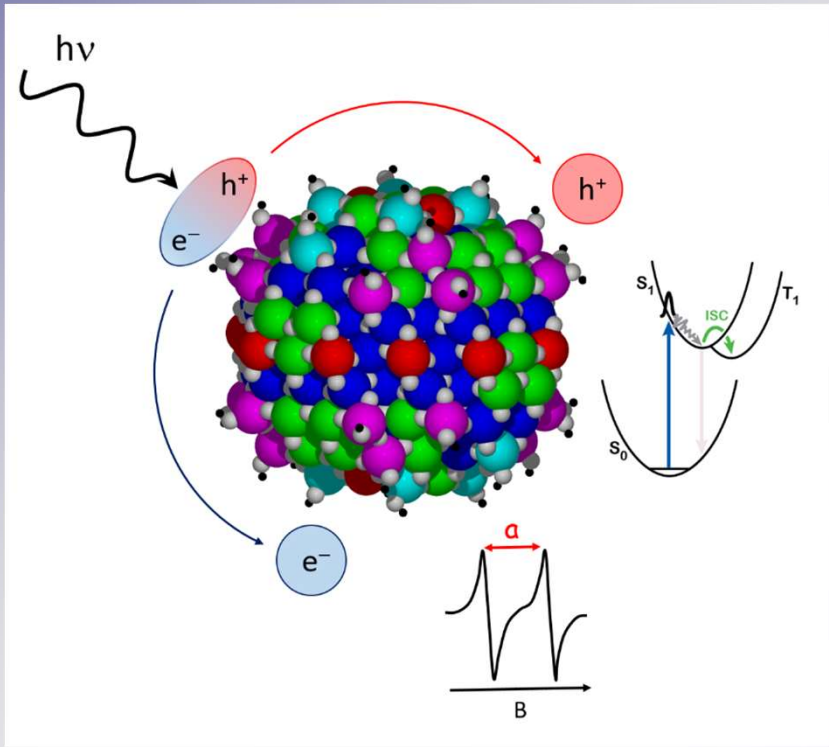


- PHOTOEXCITATION
- BULK EXCITONS
- RECOMBINATION?
- CHARGE CARRIERS SEPARATION
- ELECTRON AND HOLE TRAPPING
- MIGRATION TO THE SURFACE
- REDOX PROCESSES



COLLABORATION:
PRICETON UNIVERSITY
Annabella Selloni

CONFRONTO CON GLI ESPERIMENTI



TECNICHE SPETTROSCOPICHE:

STRUCTURAL INFORMATION:
EXAFS SPECTRA

STE EMISSION ENERGIES:
PHOTOLUMINESCENCE MEASUREMENTS

TYPE OF TRAPPING SITE:
X-RAY ABS. SPECTROSCOPY

ELECTRONIC TRANSITIONS:
TRANSIENT ABS. SPECTROSCOPY

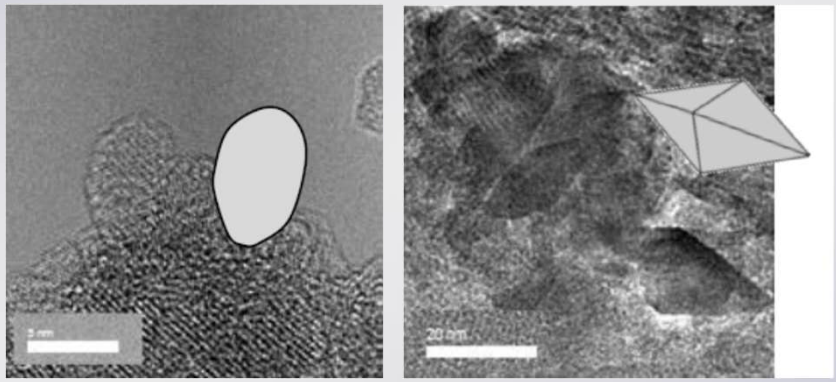
LOCALIZATION/DELOCALIZATION:
EPR SPECTROSCOPY

TRAPPING ENERGY:
IR SPECTROSCOPY

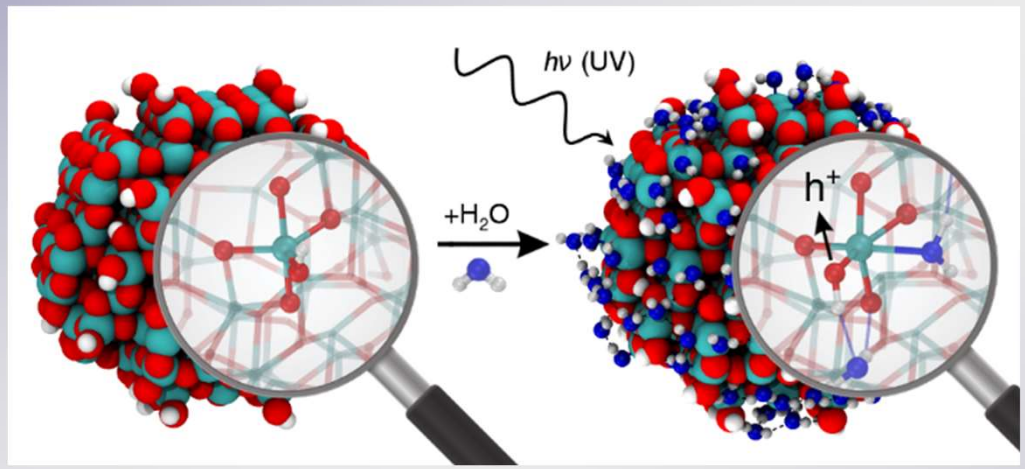
Fazio, Ferrighi, CDV *Nano Energy* 2016 27 673

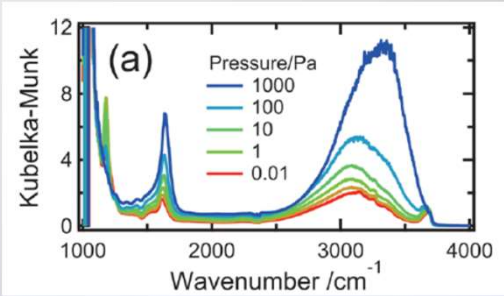
COLLABORAZIONI SPERIMENTALI

EXP. COLLABORATION:
KYOTO UNIVERSITY
Yoshiyasu Matsumoto

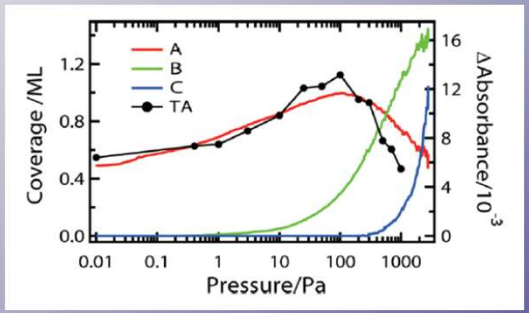


SPHERICAL 4-5 nm FACETED 10 nm





IR SPECTRA



TRANSIENT ABSORPTION

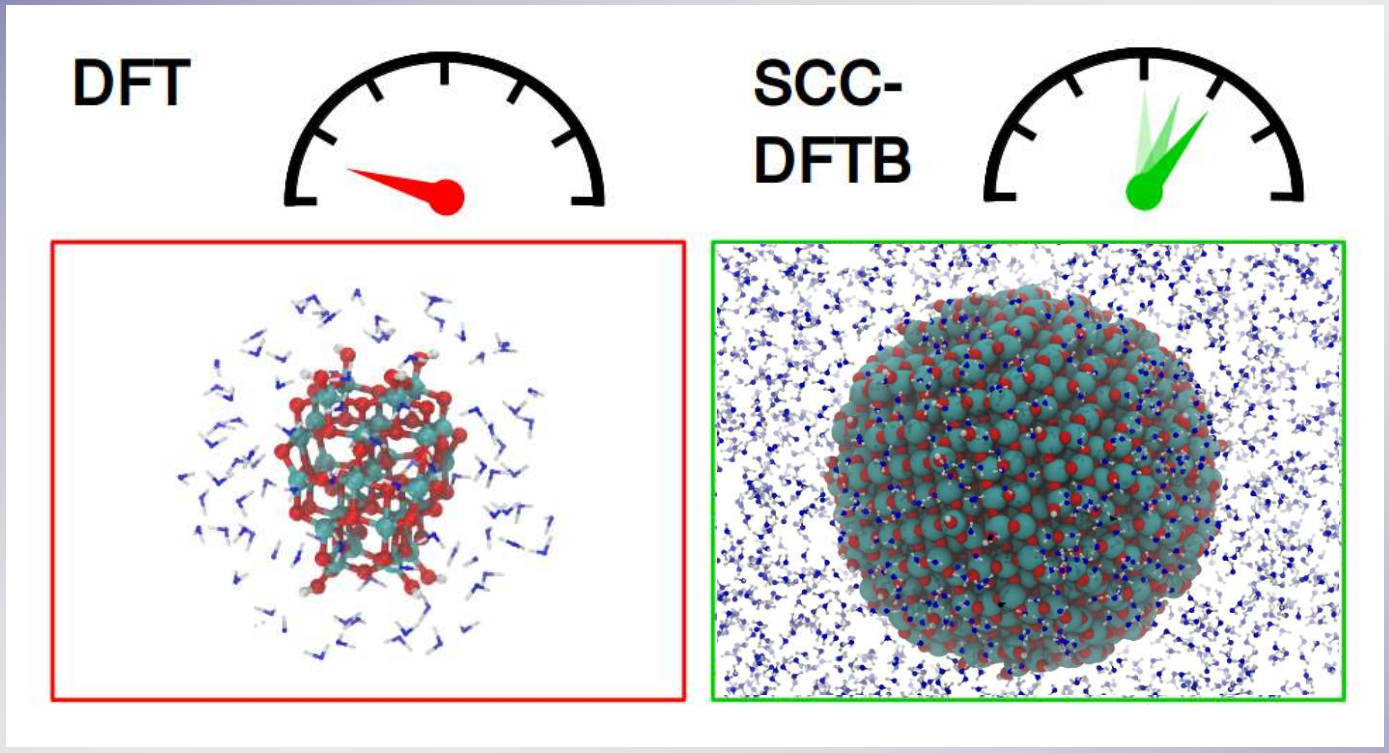
Shirai, Fazio, …, CDV, Matsumoto *JACS* 2018 140 1415

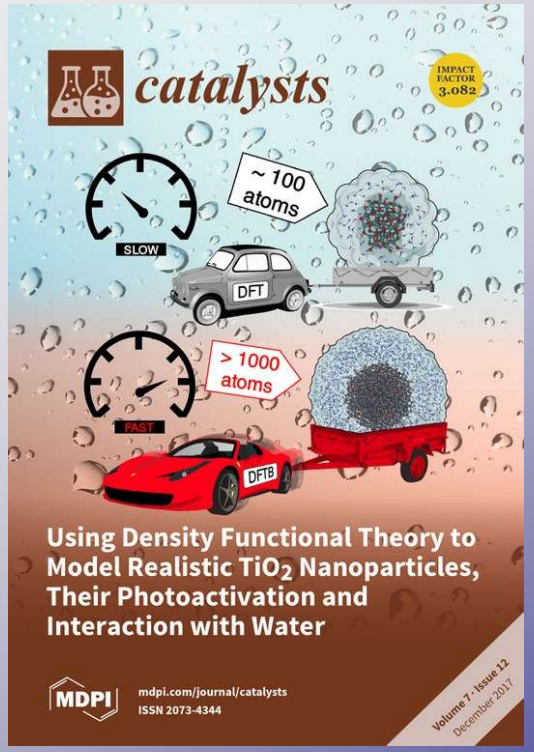
MILANO 21/10/2022

SISTEMI PIÙ GRANDI E COMPLESSI

COLLABORATION:
DRESDEN UNIVERSITY
Gotthard Seifert

TECHNISCHE UNIVERSITÄT DRESDEN

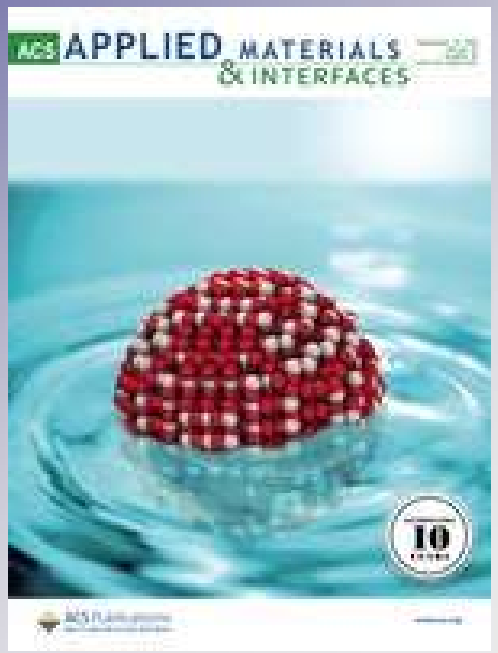


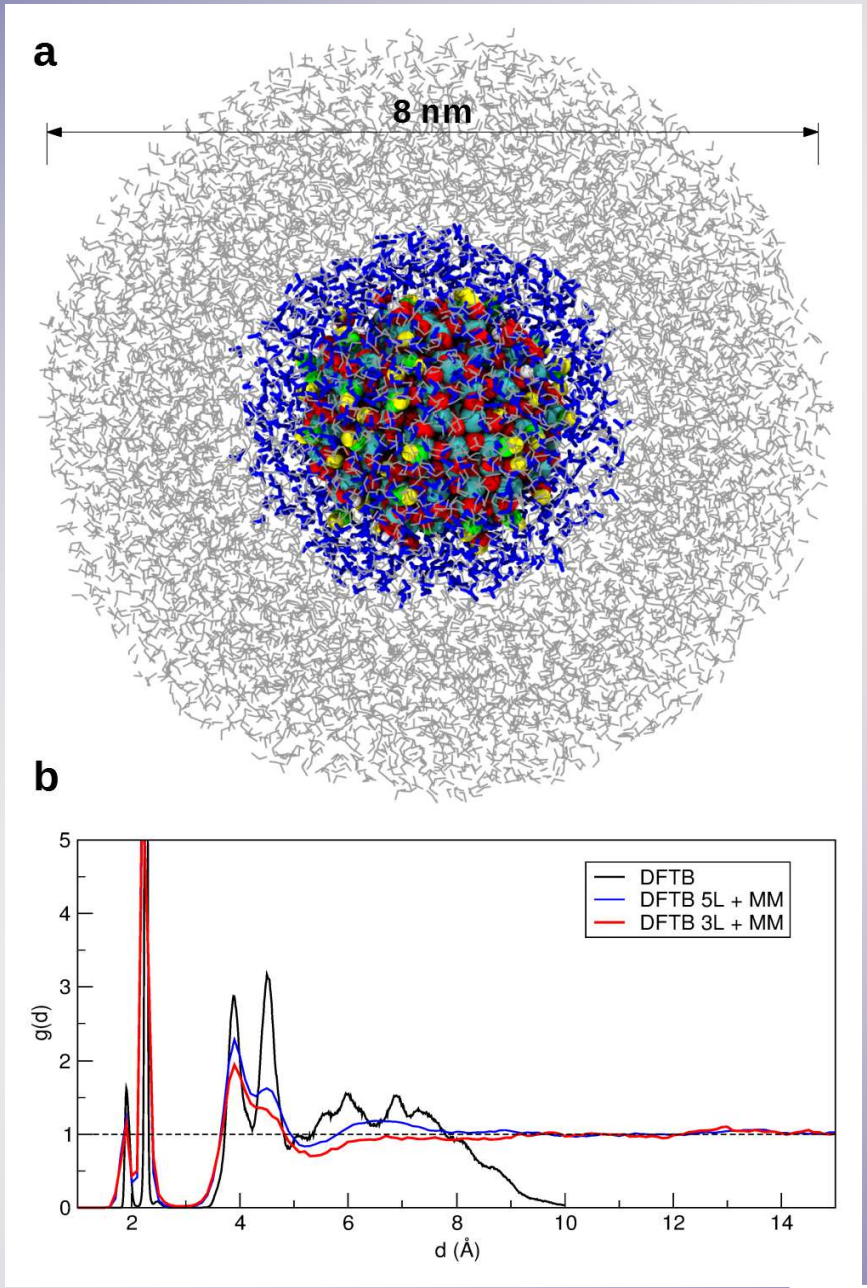


DFTB LEVEL OF THEORY

MILANO 21/10/2022

SISTEMI ANCORA PIÙ GRANDI E COMPLESSI





+8000 water molecules

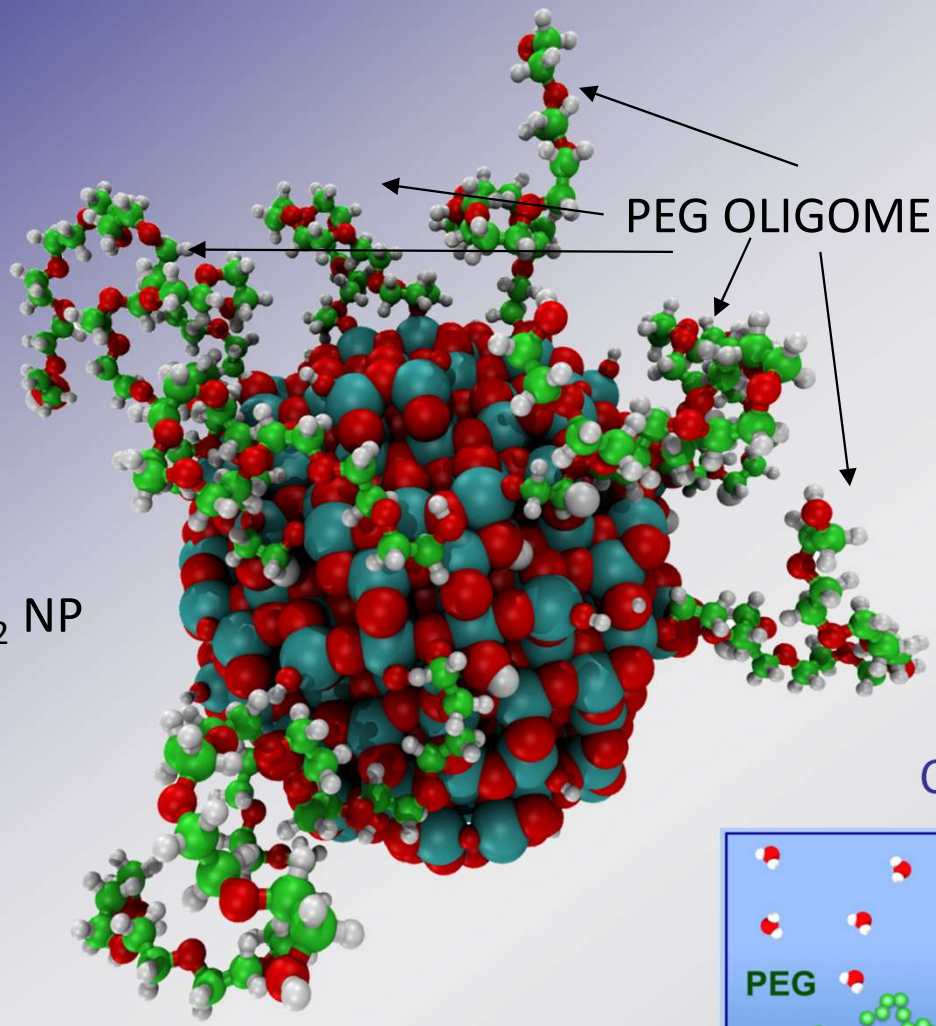
MD at 300 K

Fazio, Selli, Seifert, CDV *ACS Appl. Mater. & Interf.* **2018** 10 29943

Liu, Siani, Bianchetti, Zhao, CDV *Nanoscale* **2021** 13 9293

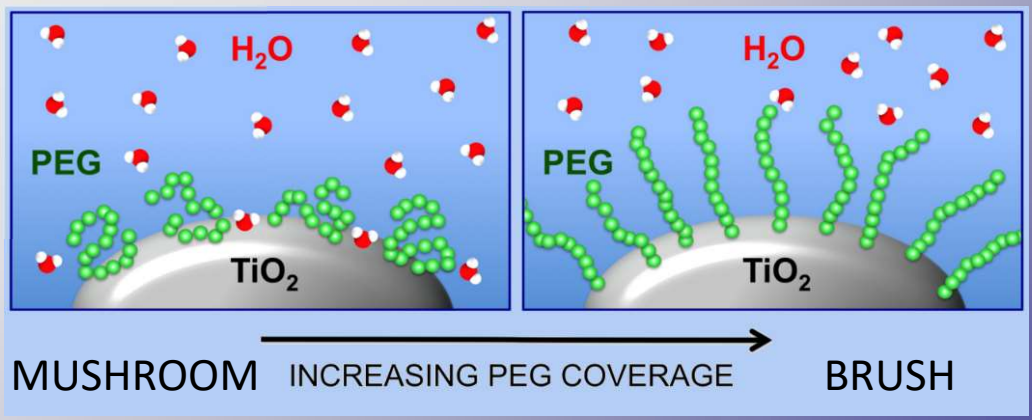
FUNZIONALIZZAZIONE

EXP. COLLABORATION:
OUR UNIVERSITY
Roberto Simonutti



TO IMPROVE
NPs BIOCOMPATIBILITY

COMPETITION WITH WATER

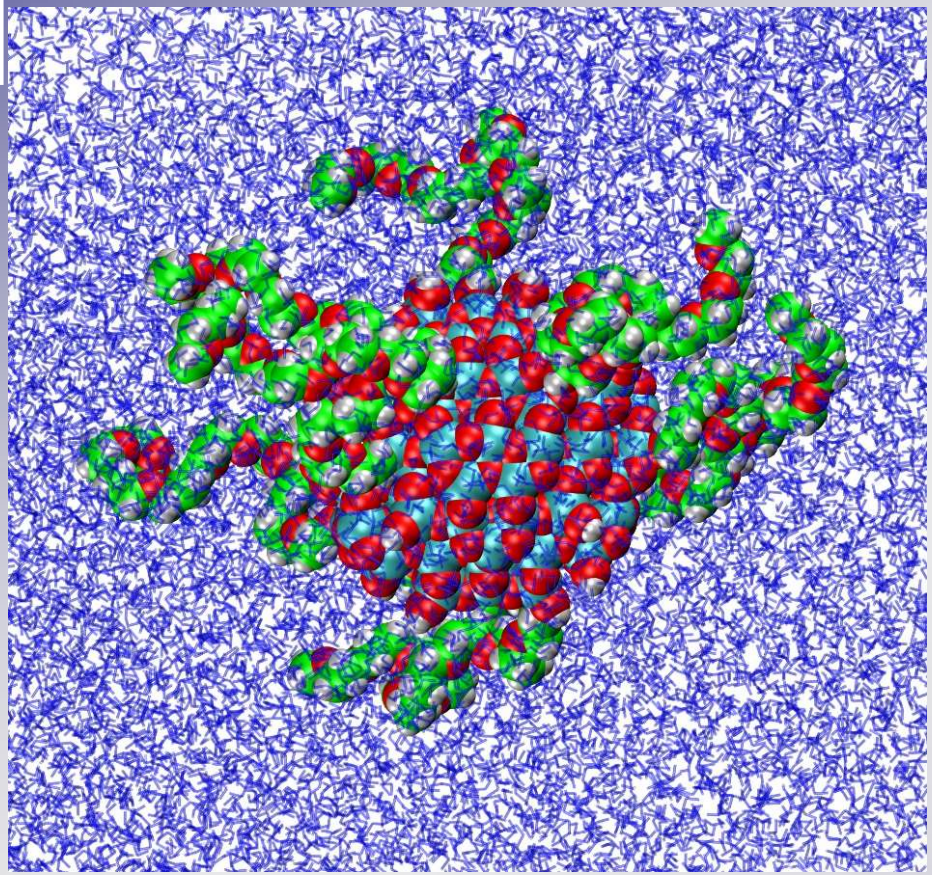


Selli, CDV *JPC C* **2016** 120 29190
Selli, Motta, CDV *J. Colloid & Interface Sci.* **2019** 555 519

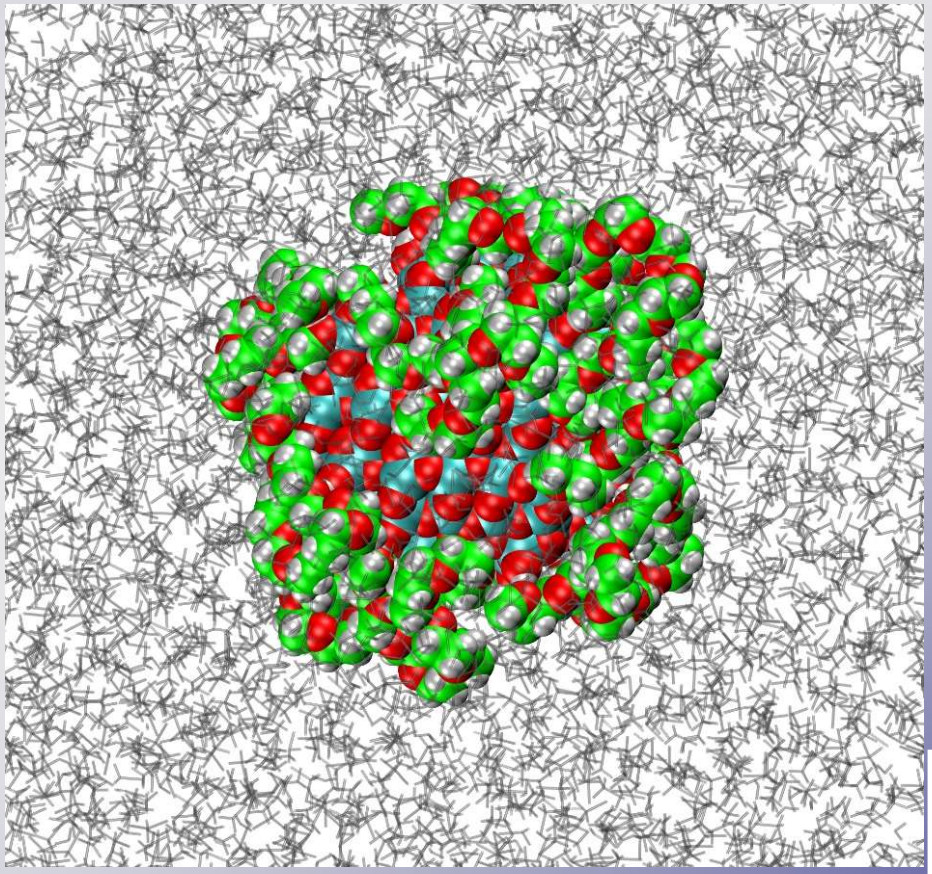
PEG COATING

MOLECULAR DYNAMICS AT 300 K

IN WATER



IN DCM



BRUSH?

MUSHROOM?

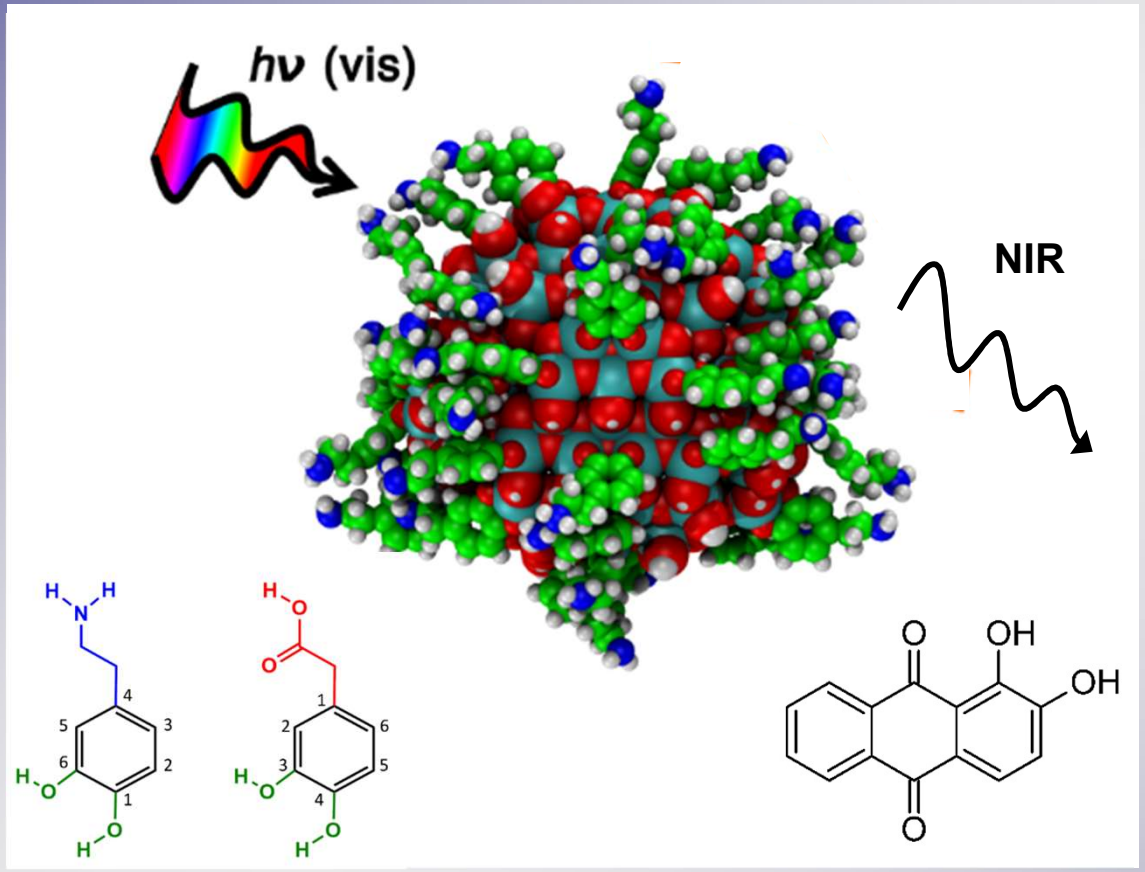
EXP. COLLABORATION:
Roberto Simonutti

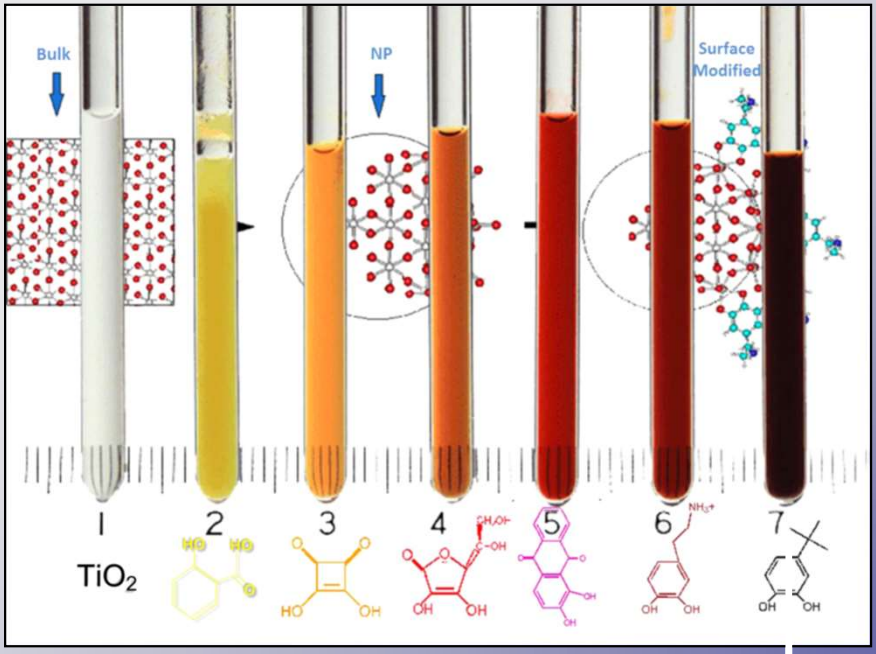
Selli, Tawfilas, Mauri, Simonutti, CDV
Chem. Mater. **2019** 31 7531

MILANO 21/10/2022

FUNZIONALIZZAZIONE

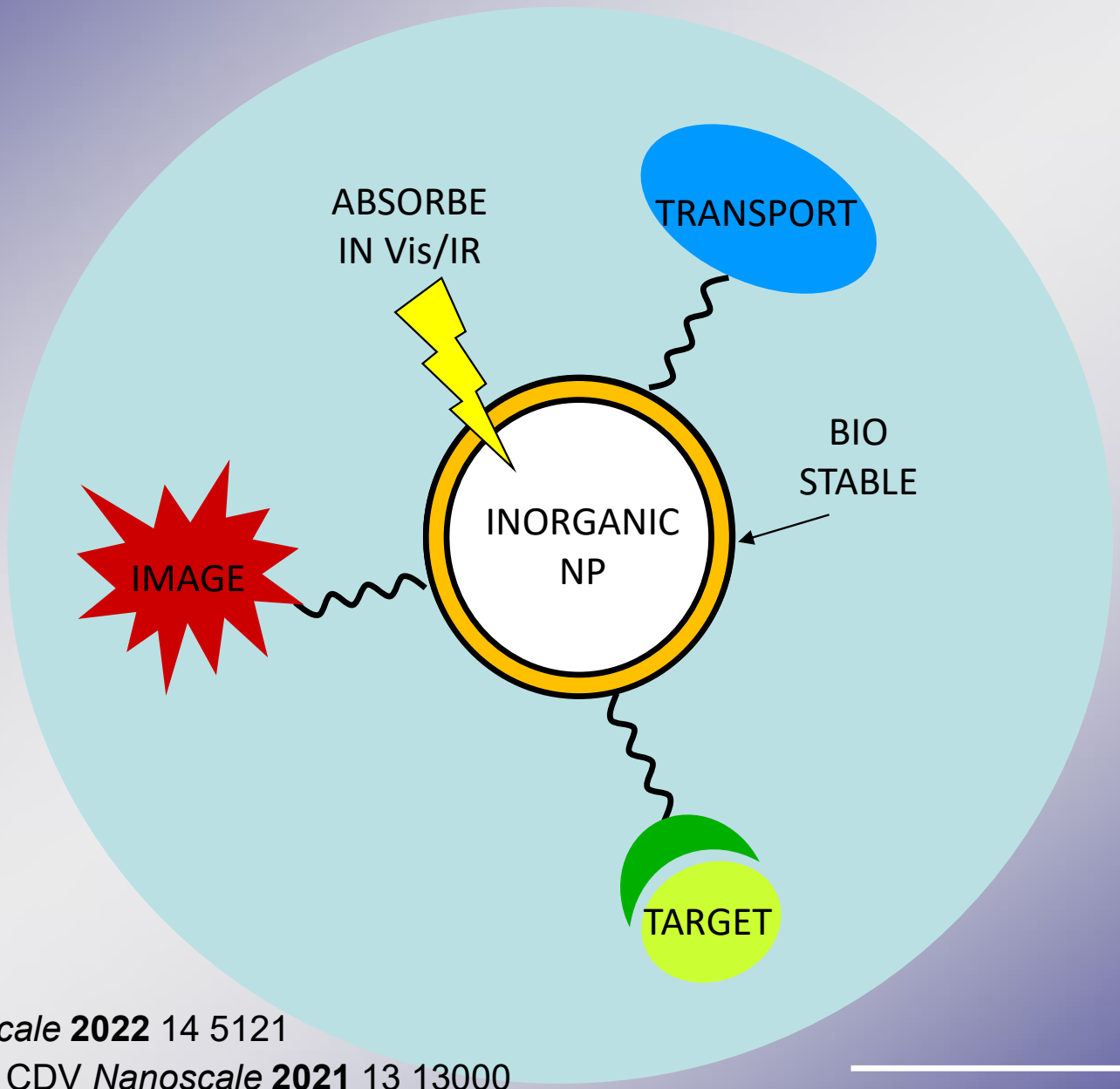
- TO MODIFY ABSORPTION REGION AND IMPROVE TISSUE PENETRATION FOR PHOTODYNAMIC THERAPY
- TO ACTIVATE FLUORESCENT PROPERTIES FOR IMAGING





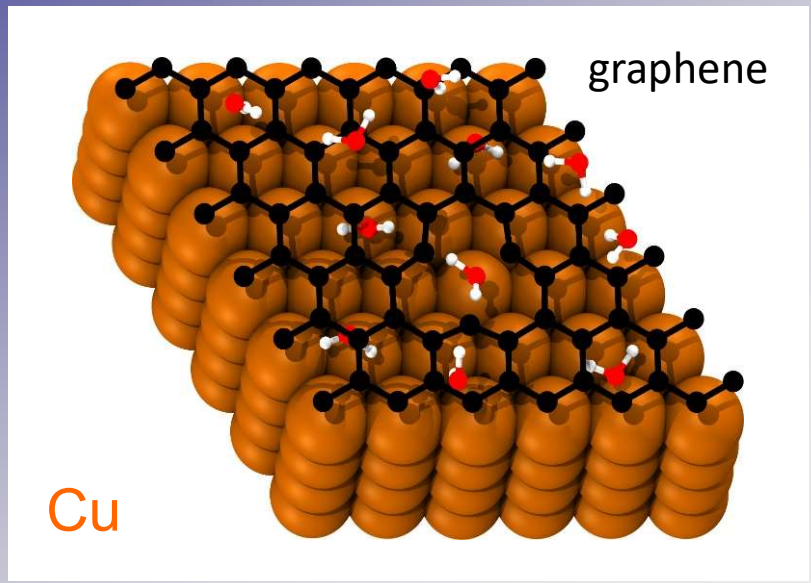
Selli, Ronchi, Pipornpong, CDV *JPC C* **2019** 123 7682
Ronchi, Datteo, Kaviani, Selli, CDV *JPC C* **2019** 123 10130
Ronchi, Soria, Ferraro, Botti, CDV *MTEnergy* **2021** 19 100571

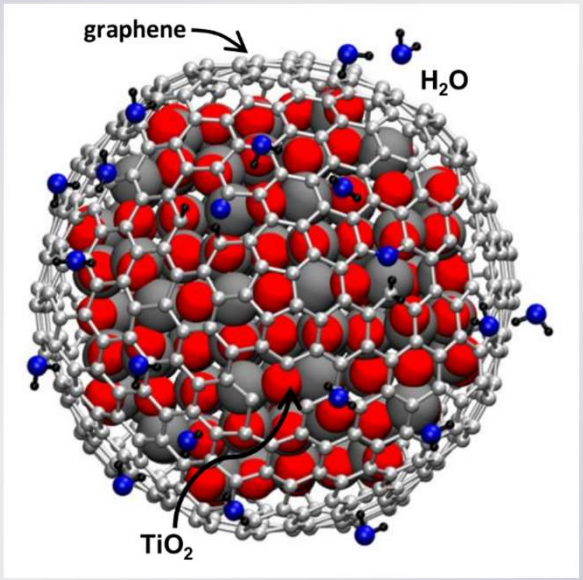
STIMULI-RESPONSIVE NANOMATERIALS

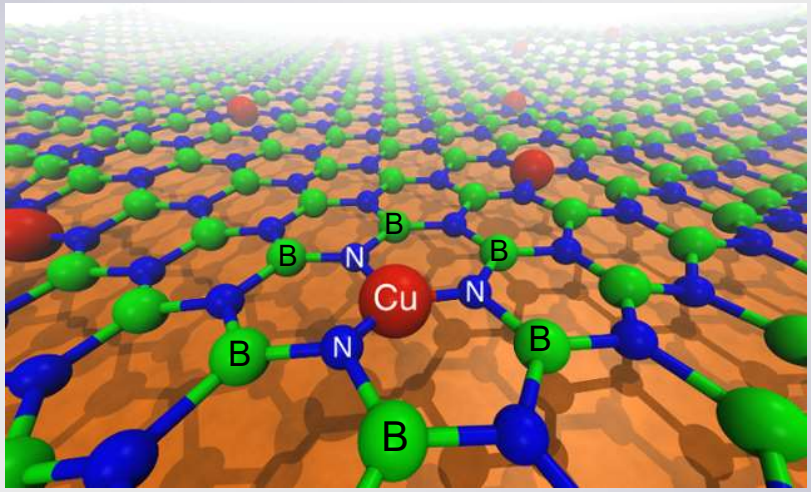


Siani, CDV *Nanoscale* **2022** 14 5121
Motta, Siani, Levy, CDV *Nanoscale* **2021** 13 13000
Donadoni, Siani, Frigerio, CDV, *Nanoscale* **2022** 14 12099

INTERFACCE CON MATERIALI 2D







h-BN/Cu(111)

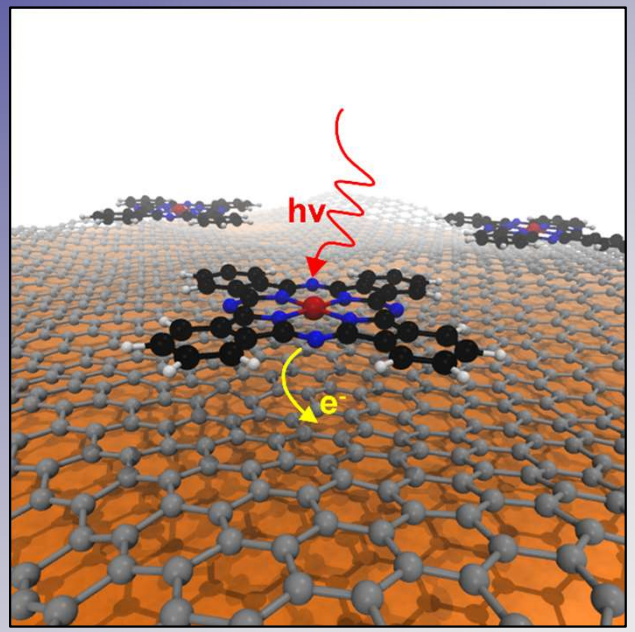
CATALYSIS UNDER COVER

CATALYSIS BY
METAL ATOMS TRAPPING

ELECTROCATALYSIS

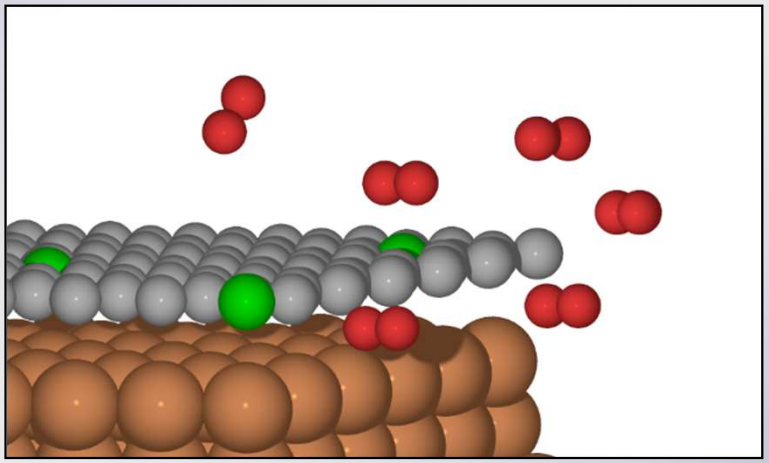
INTERFACCE CON MATERIALI 2D

MOLECULAR INTERFACES



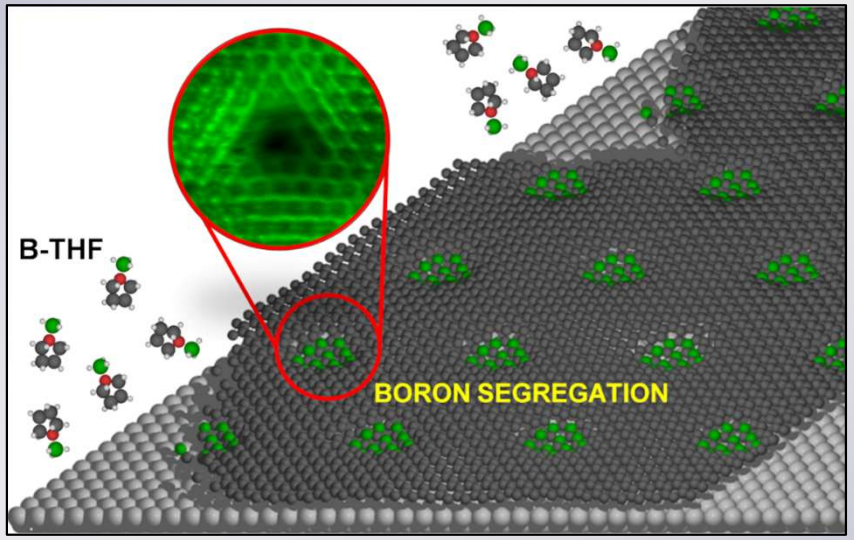
ACS Nano **2022** 16 10456

METAL INTERFACES

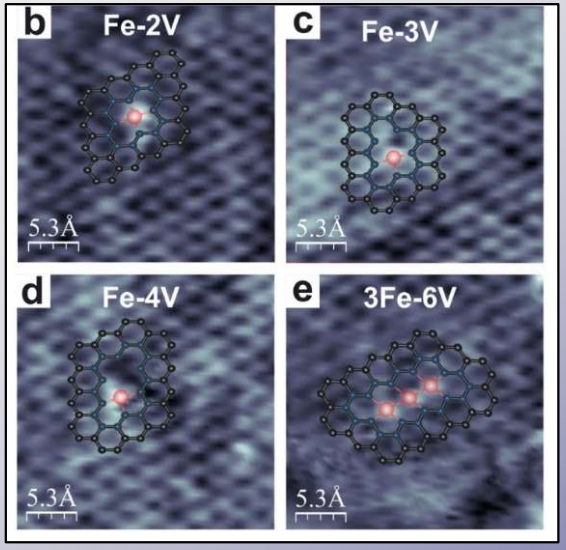


J. Am. Chem. Soc. **2016** 138 7365

DOPED GRAPHENE ON METAL SUBSTRATES

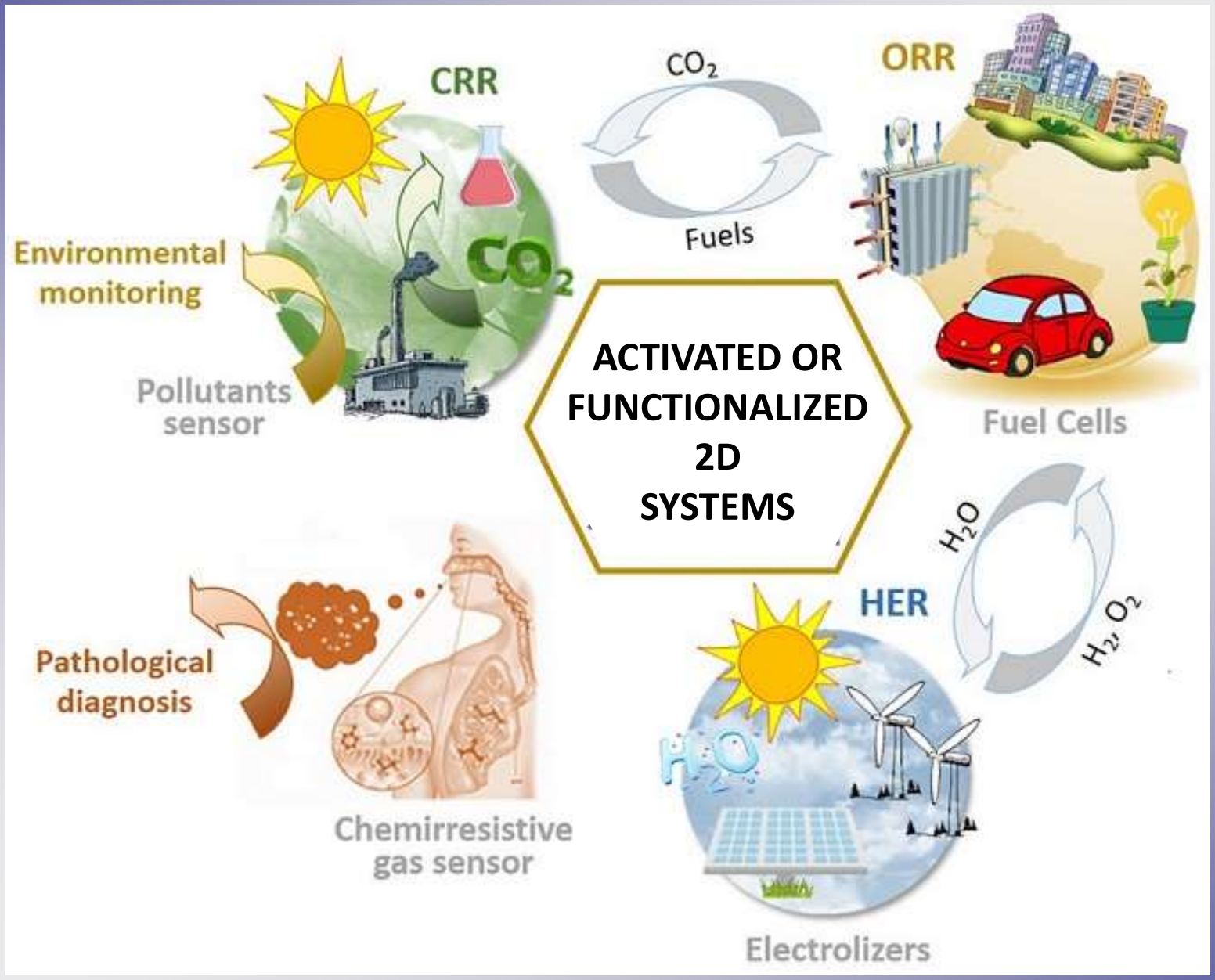


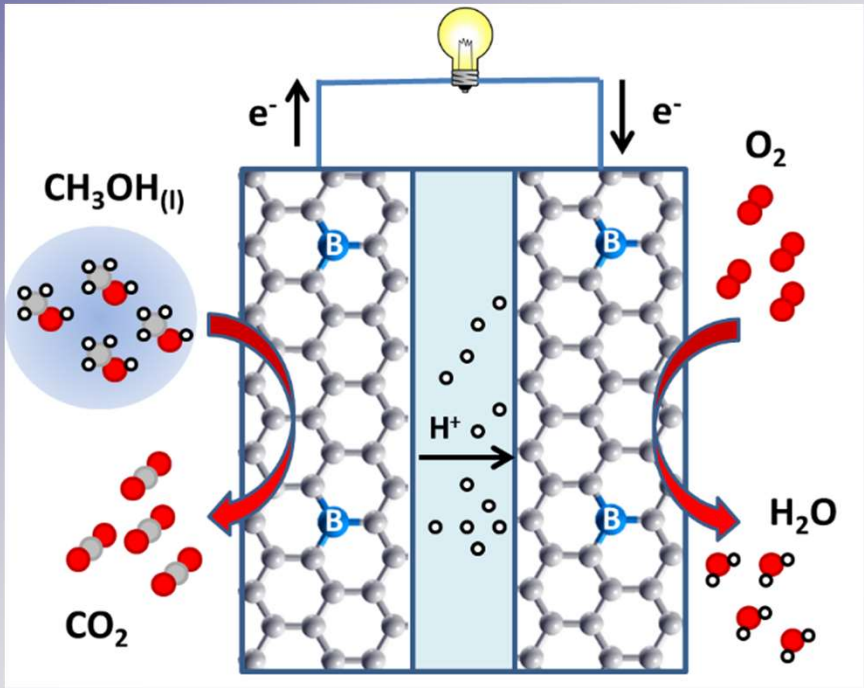
Carbon **2023** 201 881



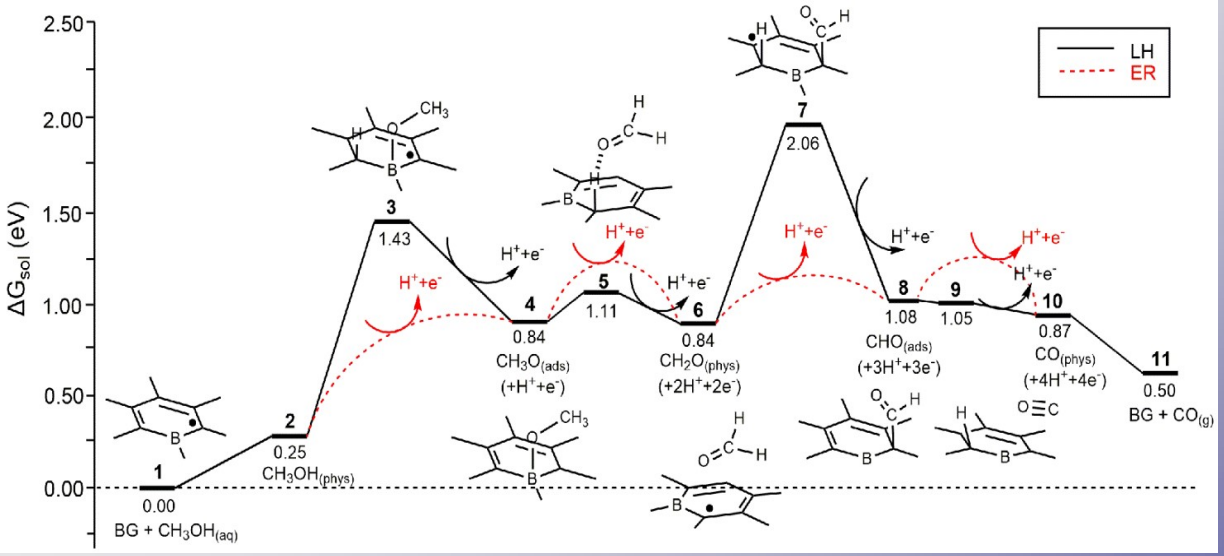
Nature Catalysis **2021** 4 850

MILANO 21/10/2022


CRR
CO_2
ORR
Environmental monitoring
CO_2
Fuels
Pollutants sensor
ACTIVATED OR FUNCTIONALIZED 2D SYSTEMS
Fuel Cells
H_2O
HER
H_2, O_2
Pathological diagnosis
H_2O
Chemirresistive gas sensor
Electrolizers



ELETTROCHIMICA COMPUTAZIONALE



Fazio, Ferrighi, CDV *J. of Catalysis* **2014** 318 203

COLLABORAZIONI

Gotthard Seifert	UNIVERSITÀ DI DRESDA GERMANIA
Annabella Selloni	PRINCETON UNIVERSITY USA
Yoshiyasu Matsumoto	UNIVERSITÀ DI KYOTO GIAPPONE
Luigi Sangaletti	UNIVERSITÀ CATTOLICA DI BRESCIA
Stefano Agnoli	UNIVERSITÀ DI PADOVA
Cristina Africh	UNIVERSITÀ DI TRIESTE
Silvana Botti	UNIVERSITÀ DI JENA
Asmus Ougaard Dohn	UNIVERSITÀ DELLA DANIMARCA
Wilhelm Auwärter	UNIVERSITÀ DI MONACO
Qiang Cui	BOSTON UNIVERSITY

www.nanoQlab.mater.unimib.it

PRIN 2022 PNRRPRIN 2022 PNR | schema_prin.docx - Documenti C | Department of Materials Science

https://www.nanoqlab.mater.unimib.it

Sincronizzazione non in corso

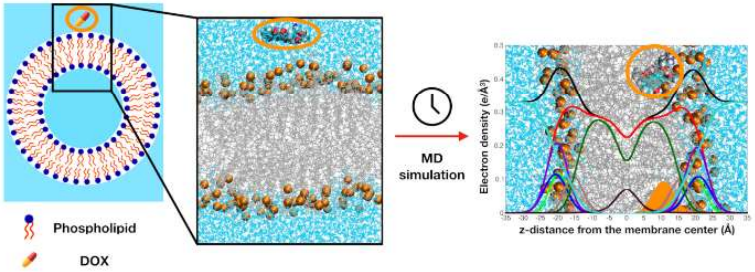
nanoQlab

Home Research People Equipment Publications Collaborations Funding

nanoQlab News Contact

Computational laboratory for
the investigation of nanosized systems
for health, energy and environment

coordinated by Cristiana Di Valentin



BBA - Biomembranes 2022, 1864, pp 183763

News

CECAM Poster Award

May 20 2022: PhD student Edoardo Donadoni has

Grazioli Prize 2021

February 17 2022: PhD student Edoardo Donadoni

Master Exam

October 28 2021: Mirko Dolce received his Master's

Scrivi qui per eseguire la ricerca

ITA 18:13 21/10/2022