

TESI DI LAUREA TRIENNALE  
E DI LAUREA MAGISTRALE  
PRESSO IL **NANOQLAB**

Prof. CRISTIANA DI VALENTIN



- DIPARTIMENTO DI SCIENZA DEI MATERIALI U5 Milano
- CENTRO DI BIONANOMEDICINA U28 Monza

UNIVERSITÀ DI MILANO-BICOCCA







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**QUESTO È L'UFFICIO DEI NOSTRI SOGNI!**



LABORATORIO  
DI CHIMICA QUANTISTICA  
PER LA NANOMEDICINA

COORDINATO DA: CRISTIANA DI VALENTIN  
HPC SPECIALIST: LORENZO FERRARO

CENTRO DI NANOMEDICINA  
MILANO BICOCCA  
MONZA



X86/CPU ARCHITECTURE

60 TFLOPS

1500 cores

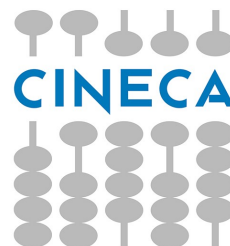
Xeon processors 2.6 GHz

7.5 TB RAM

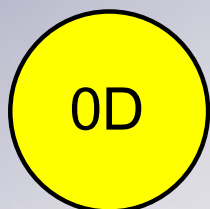
Infiniband 56 Gbit/s

STORAGE 150 TB RAW

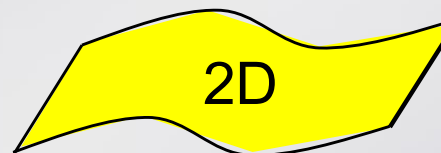
Integrated cooling systems



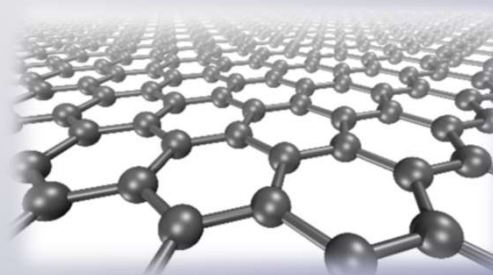
# STUDI DI CHIMICA COMPUTAZIONALE DI MATERIALI NANODIMENSIONATI E NANOSTRUTTURATI



NANOPARTICELLE



MATERIALI BIDIMENSIONALI  
G - GO - hBN - WSe<sub>2</sub> - C<sub>3</sub>N<sub>4</sub>



ALMENO UNA DIMENSIONE NELLA SCALA NANOMETRICA

PER **MEDICINA – ENERGIA – CATALISI – SENSORISTICA**



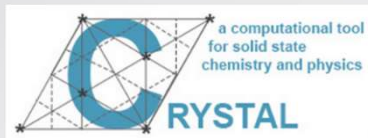
## Quantum Mechanical Methods

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

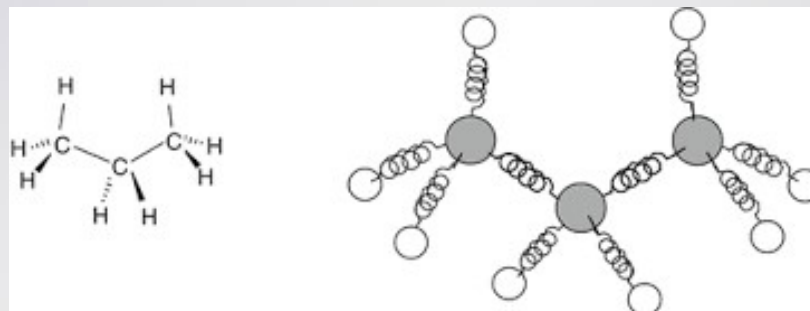
*Kinetic Energy* + *Potential Energy* = *Total Energy*



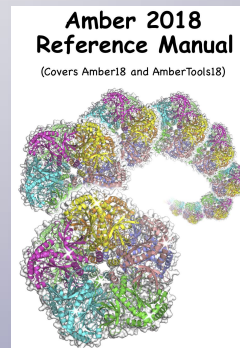
but accurate



## Molecular Mechanics Methods



but less accurate



Quantum Mechanical  
Methods

+

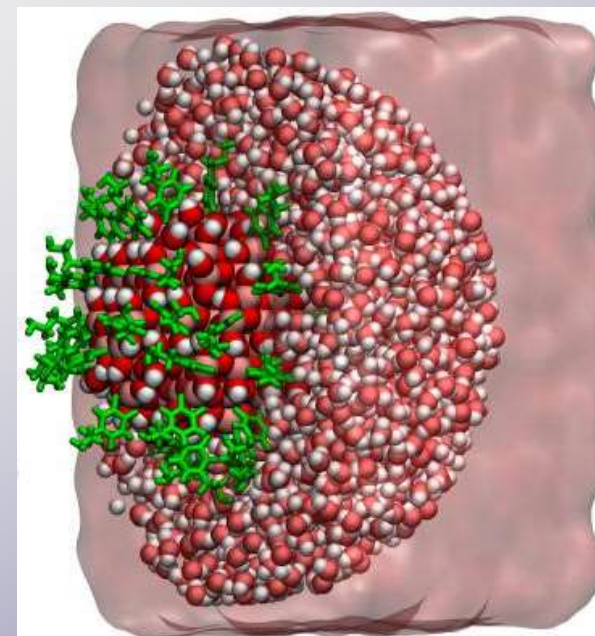
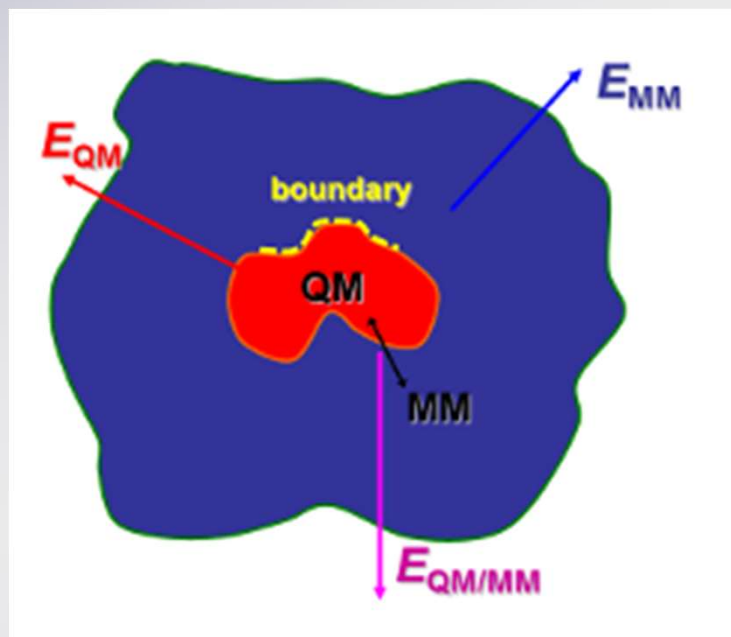
Molecular Mechanics  
Methods



QM / MM

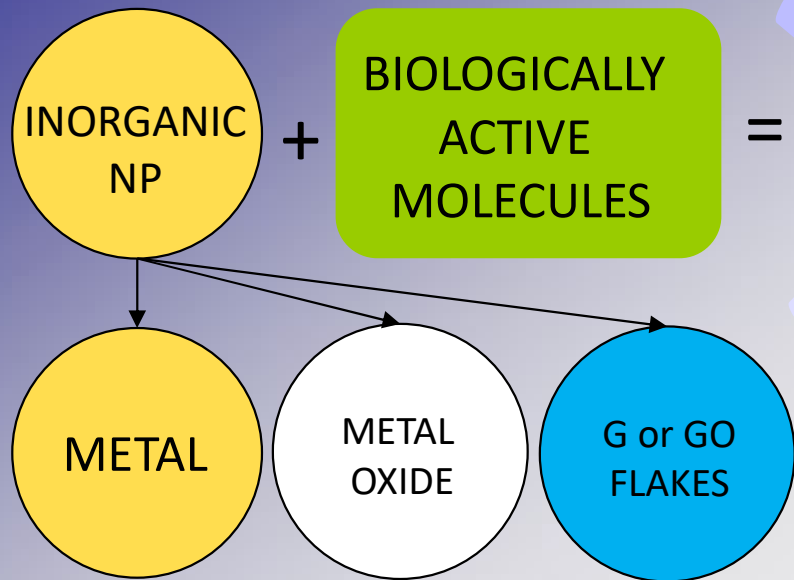
Amber 2018  
Reference Manual

(Covers Amber18 and AmberTools18)



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

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



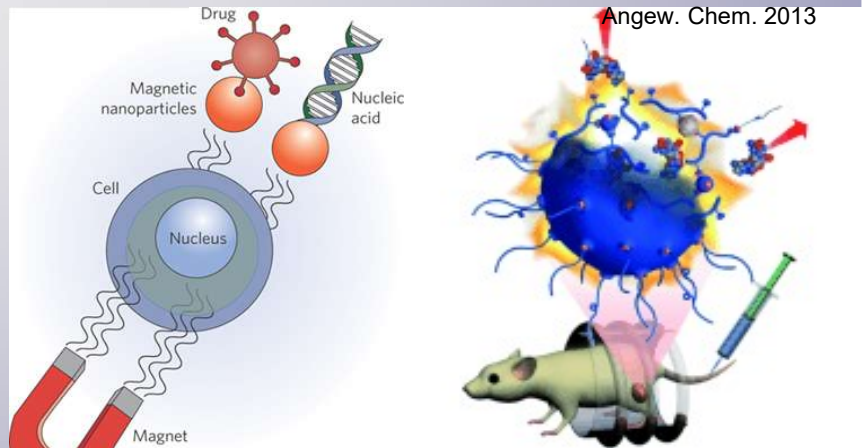
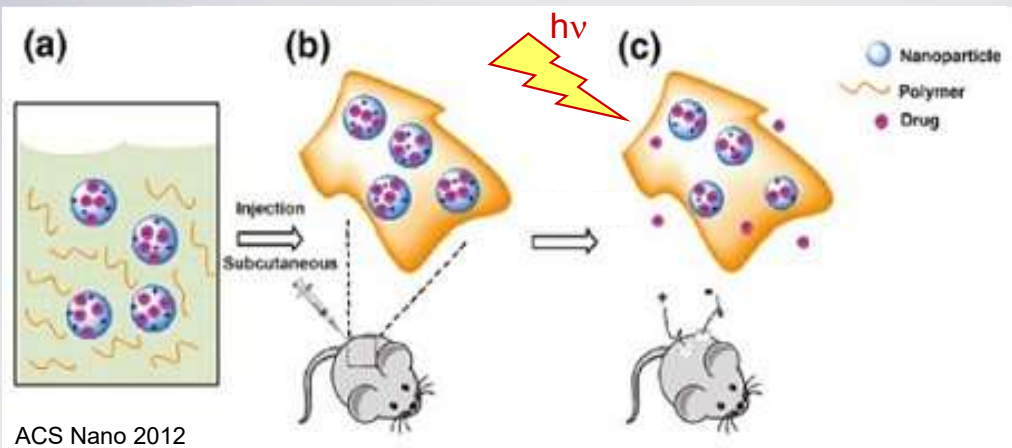
**BIOMIMESIS – TARGETING –  
DRUG DELIVERY –  
THERAPEUTICS – IMAGING**



**TERAPIA FOTODINAMICA ( $TiO_2$ )**



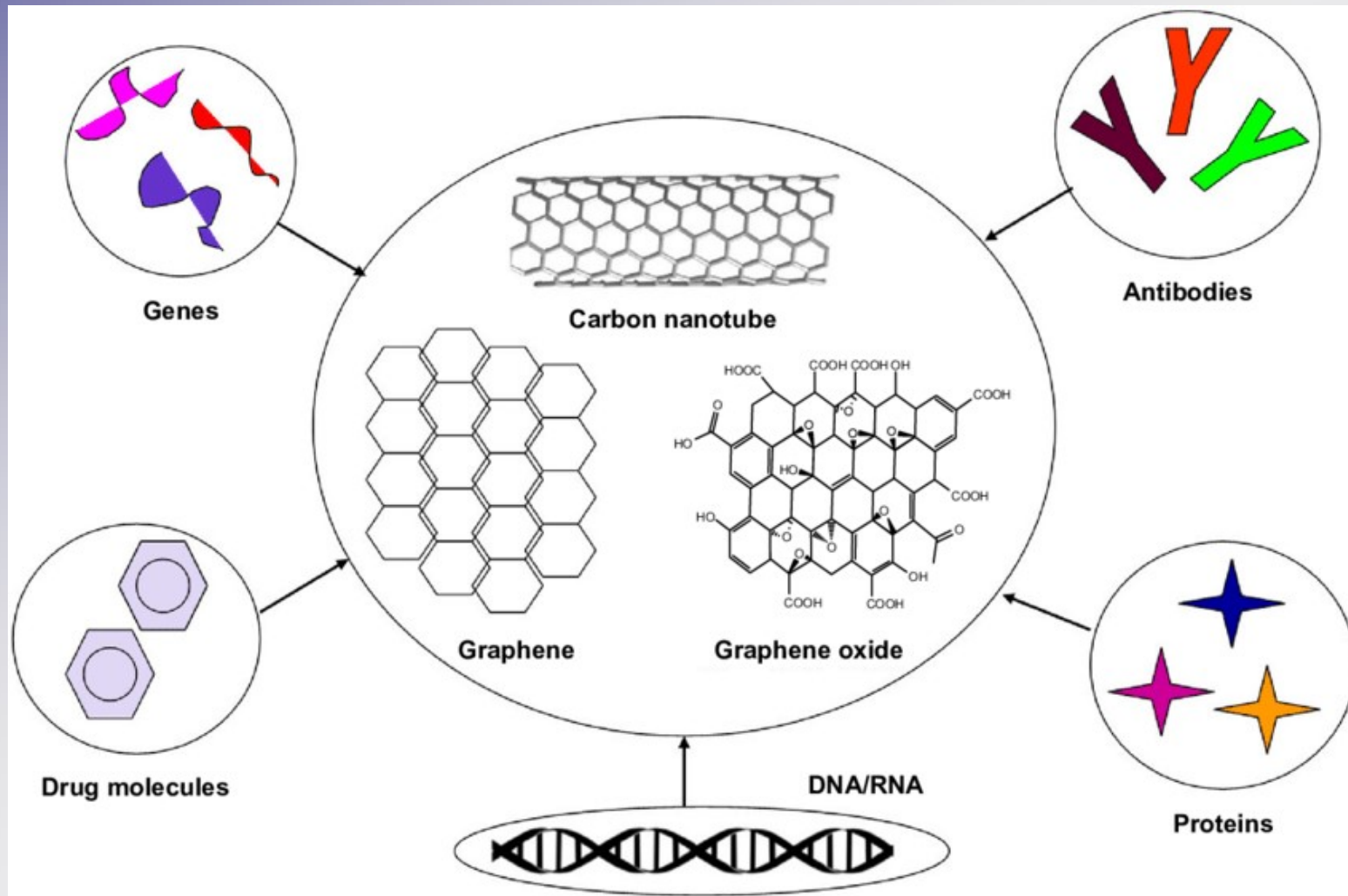
**MAGNETISMO (OSSIDI DI FERRO)**



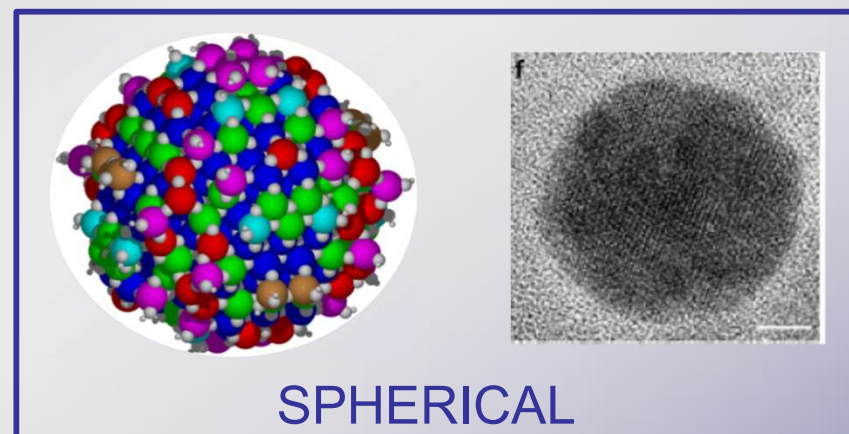
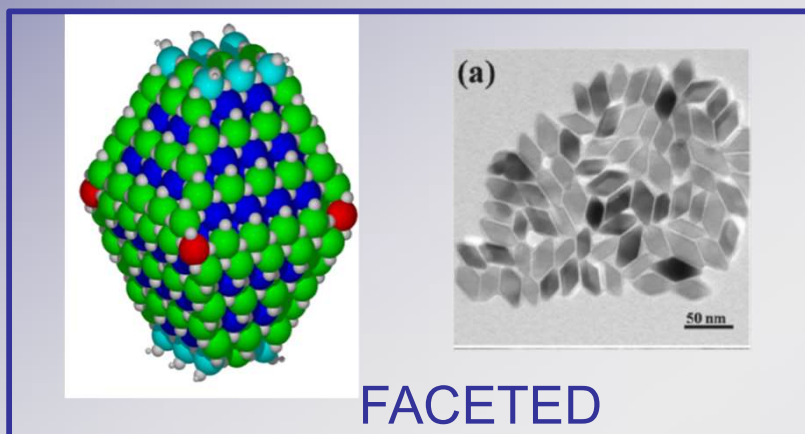
**SMART STIMULI-RESPONSIVE NANODEVICES**



## VETTORI PER TRASPORTO

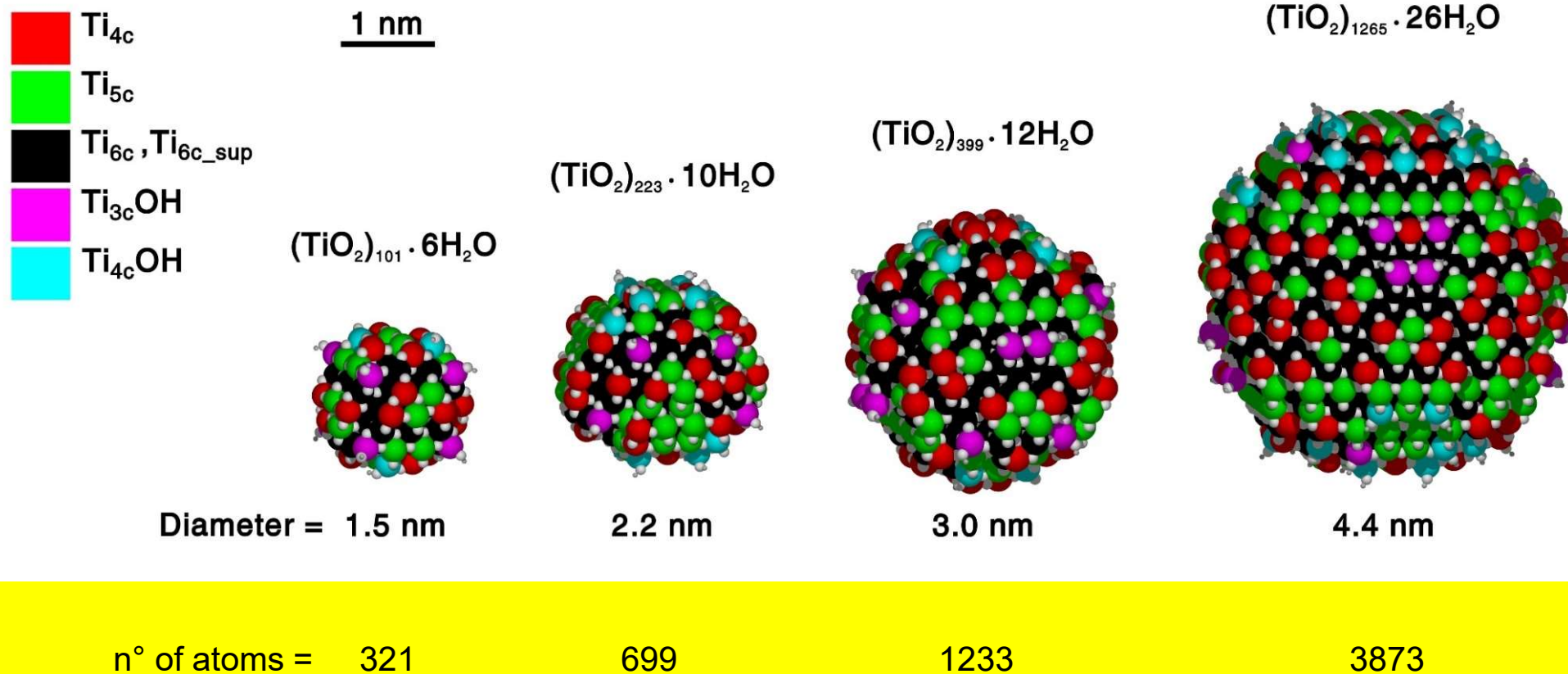


## NANOPARTICELLE DI $\text{TiO}_2$

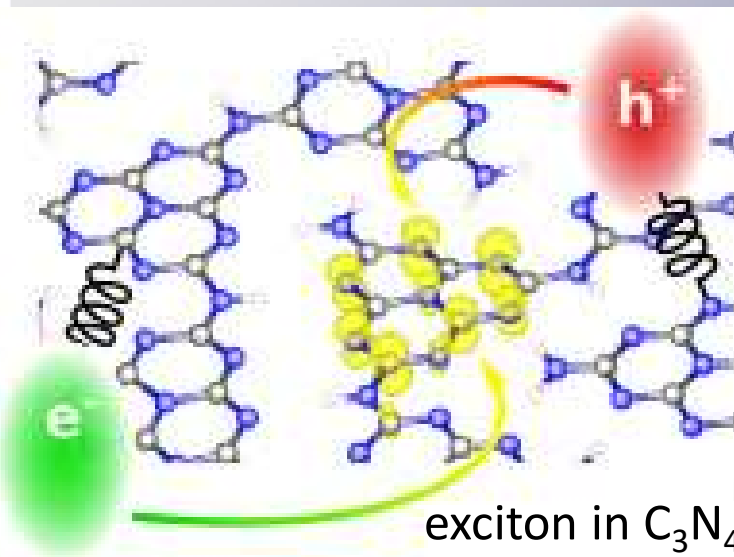
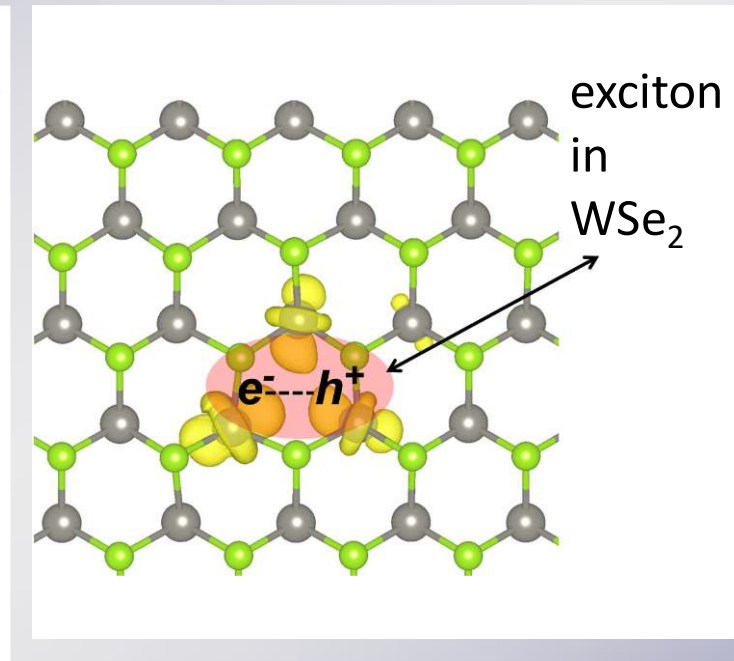
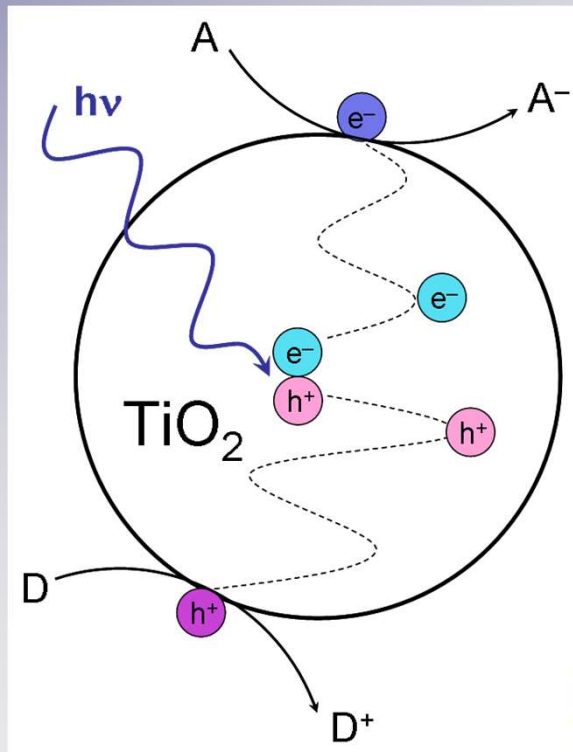
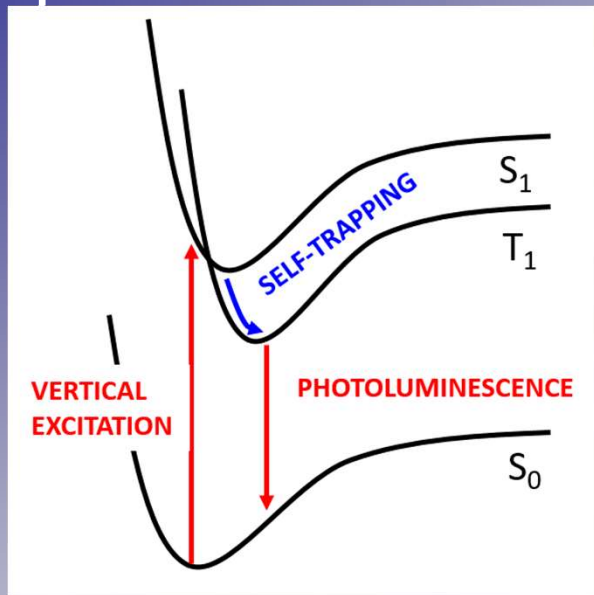


WULFF SHAPE PREDICTION:  
**DECAHEDRON**  
by Barnard et al. Nano Lett. 2005

LOW PARTICLE DENSITY



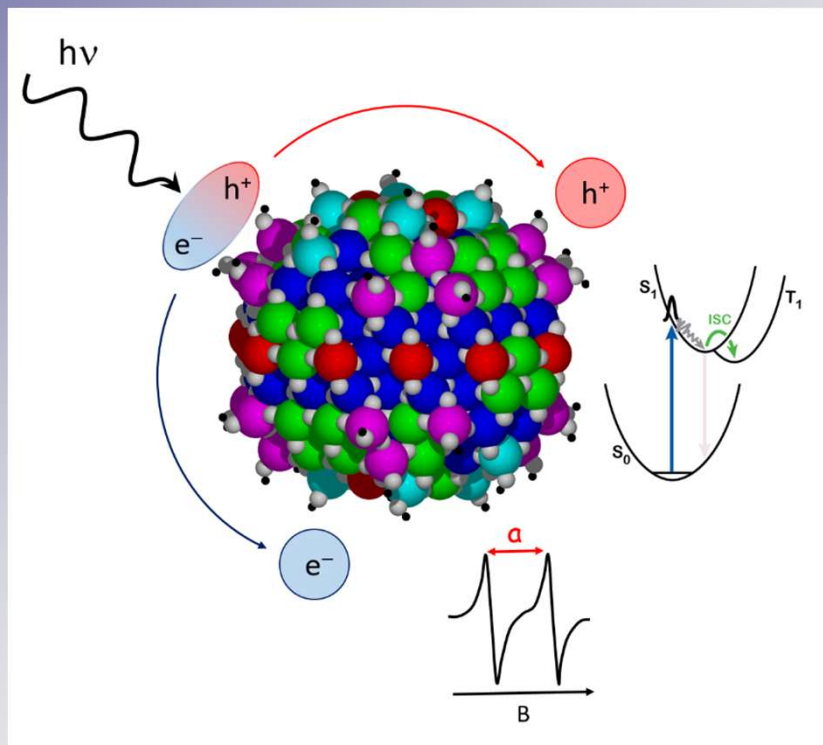




- PHOTOEXCITATION
- BULK EXCITONS
- RECOMBINATION?
- CHARGE CARRIERS SEPARATION
- ELECTRON AND HOLE TRAPPING
- MIGRATION TO THE SURFACE
- REDOX PROCESSES



COLLABORATION:  
PRINCETON UNIVERSITY  
Annabella Selloni



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:

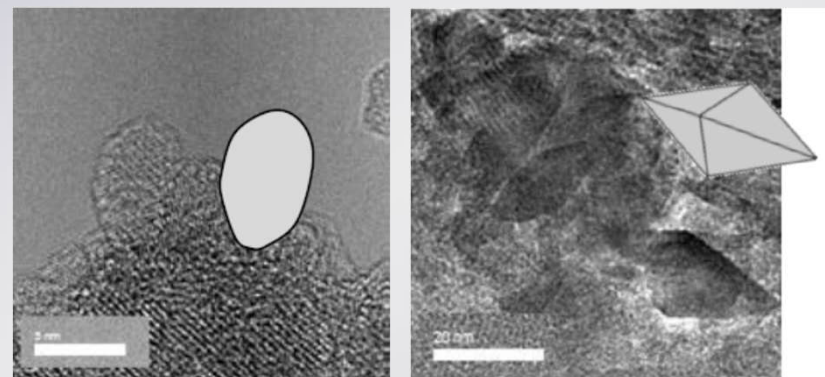
EPR SPECTROSCOPY

TRAPPING ENERGY:

IR SPECTROSCOPY

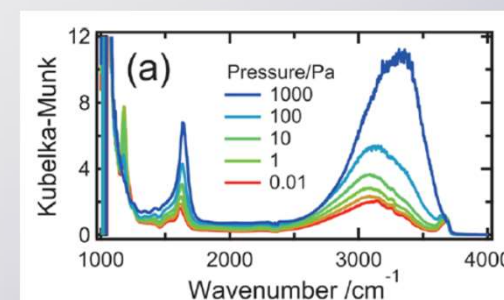
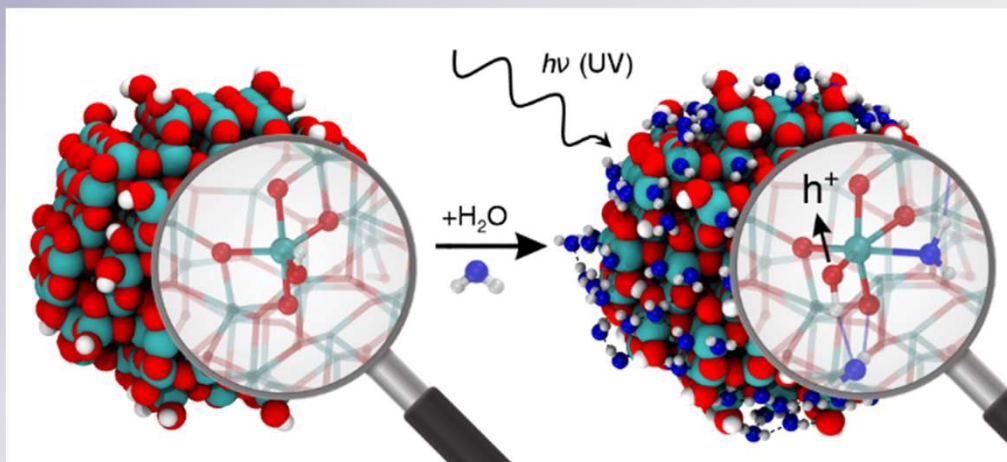


**EXP. COLLABORATION:  
KYOTO UNIVERSITY  
Yoshiyasu Matsumoto**

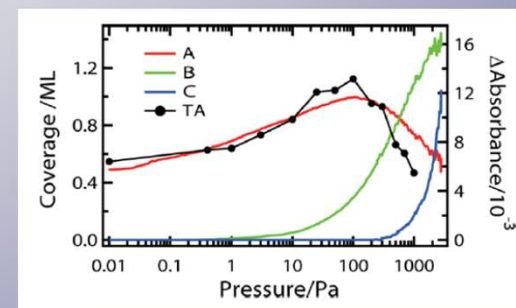


SPHERICAL 4-5 nm

FACETED 10 nm



IR SPECTRA



TRANSIENT ABSORPTION

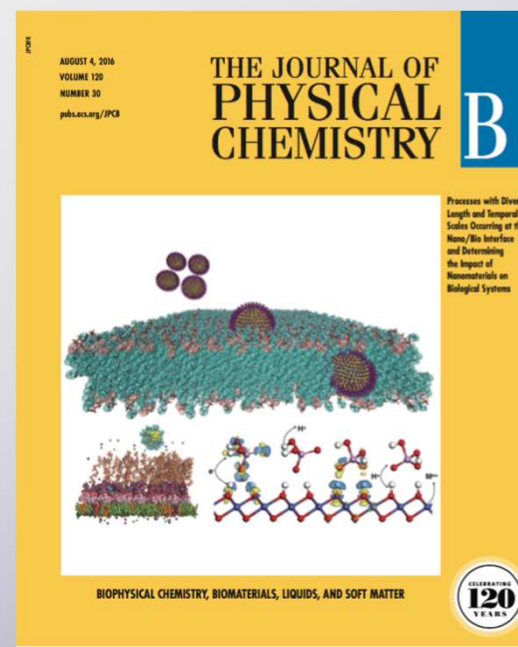
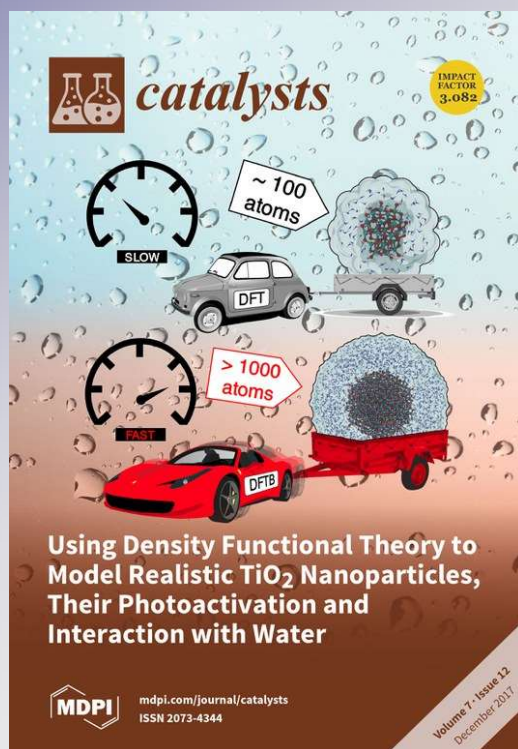


# SISTEMI PIÙ GRANDI E COMPLESSI

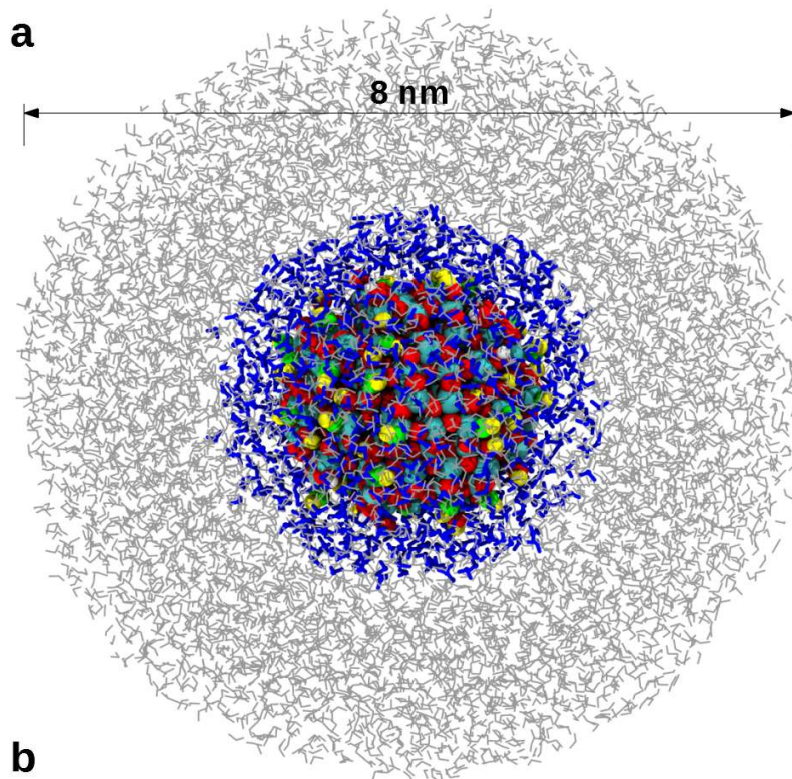
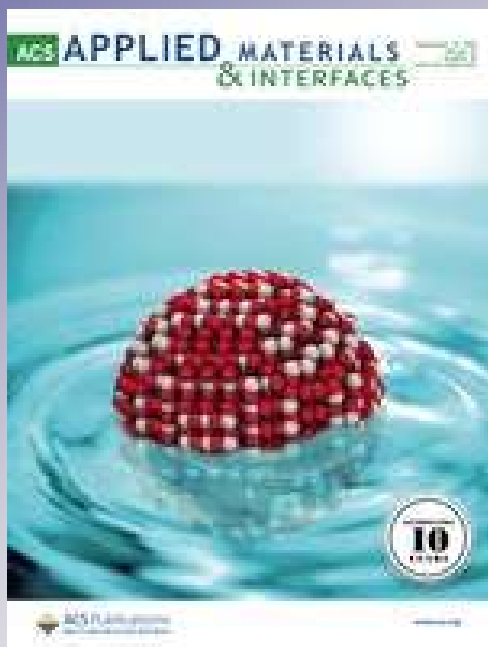
COLLABORATION:  
DRESDEN UNIVERSITY  
Gotthard Seifert



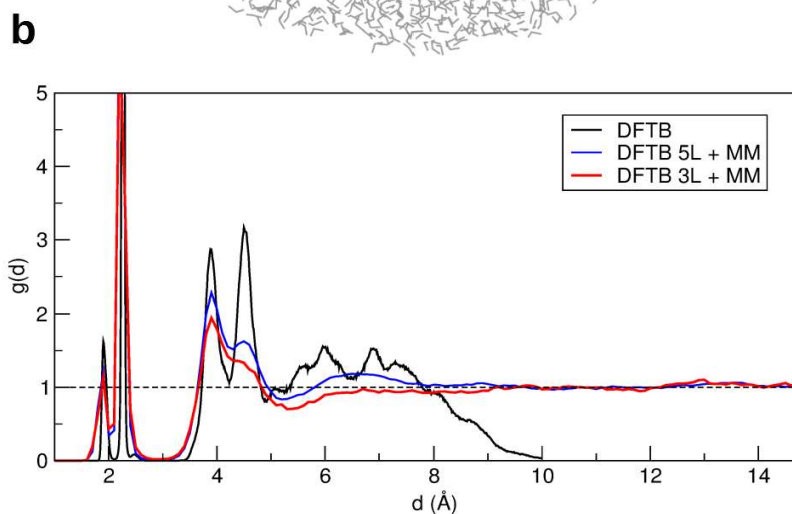
COLLABORATION:  
BOSTON UNIVERSITY  
Qiang Ciu



MILANO 16/01/2023



+8000  
water  
molecules



MD at 300 K

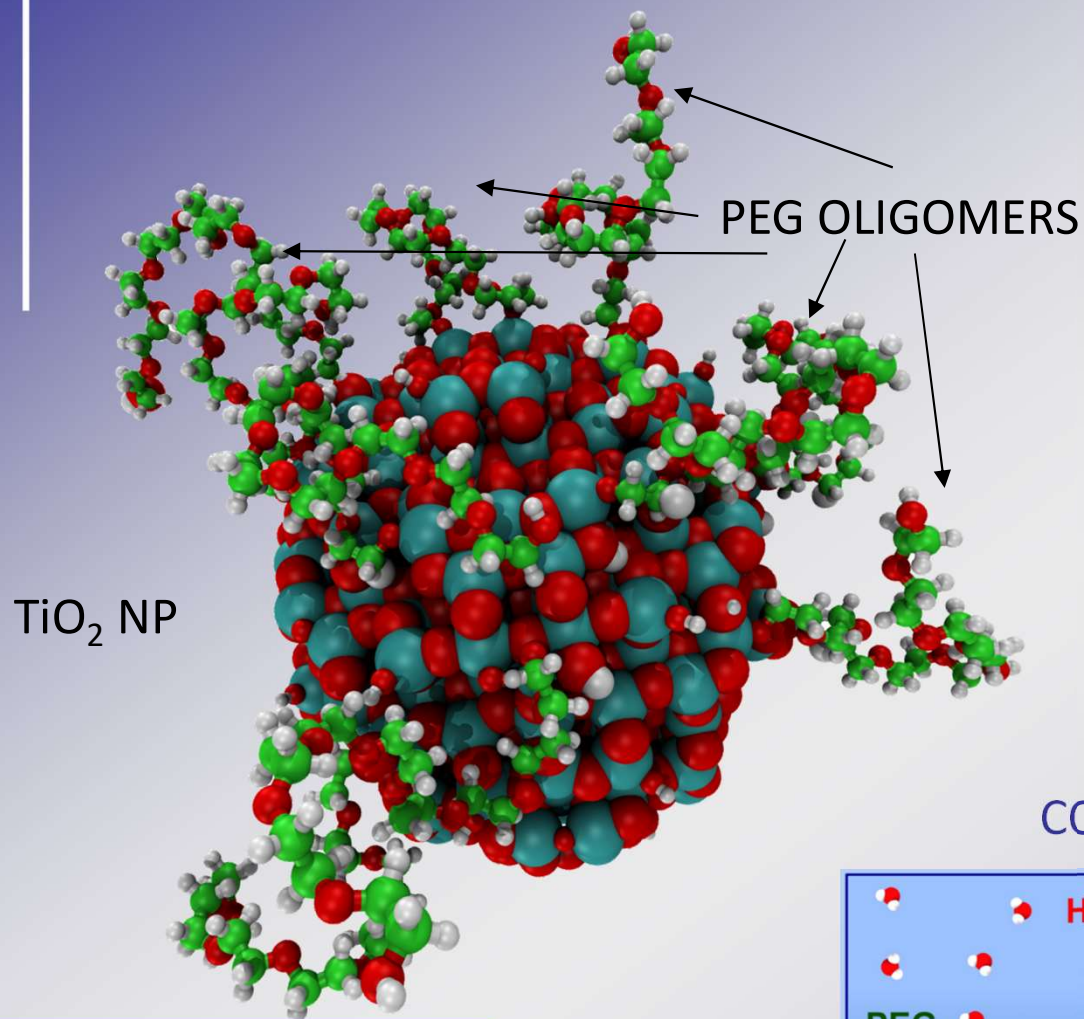
Fazio, Selli, Seifert, CDV *ACS Appl. Mater. & Interf.* **2018** 10 29943

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

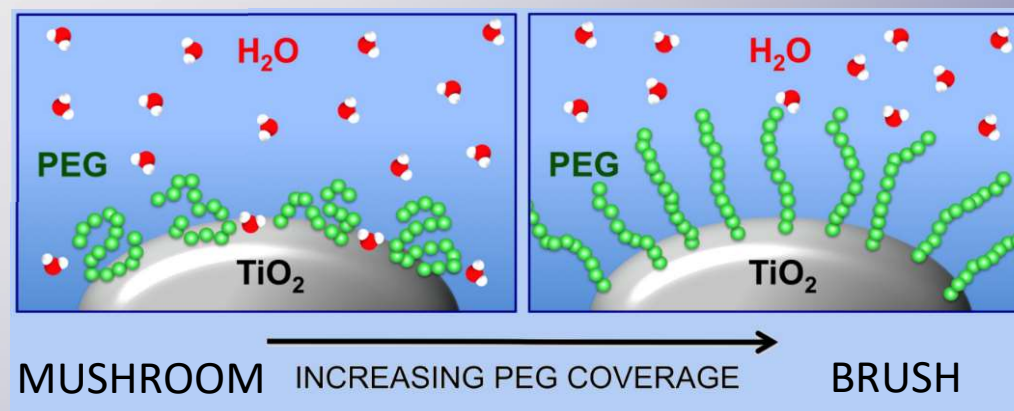
MILANO 16/01/2023



TO IMPROVE  
NPs BIOCOMPATIBILITY  
AND IN VIVO CIRCULATION TIME



COMPETITION WITH WATER



EXP. COLLABORATION:  
OUR UNIVERSITY  
Roberto Simonutti



Selli, CDV *JPC C* **2016** 120 29190

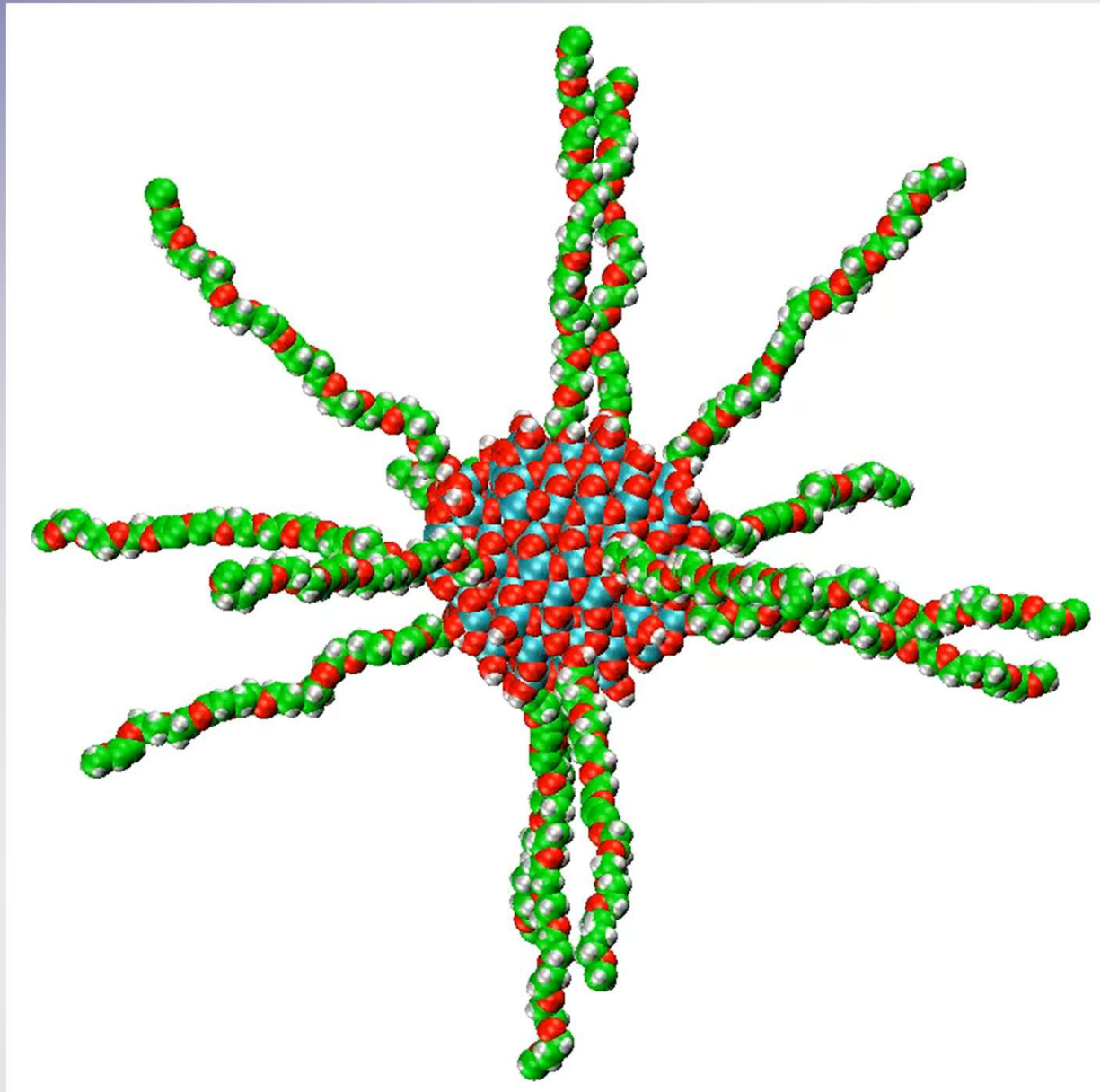
Selli, Motta, CDV *J. Colloid & Interface Sci.* **2019** 555 519

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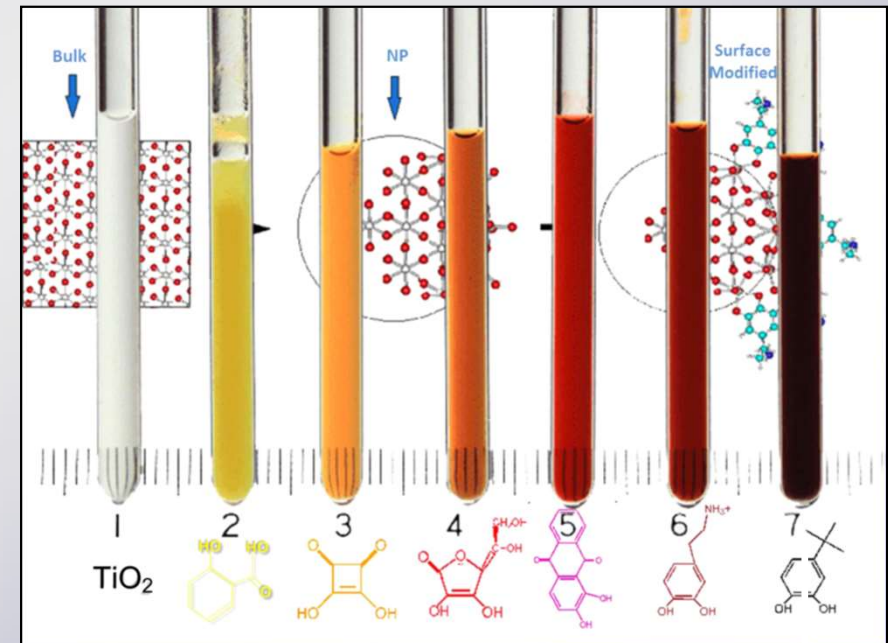
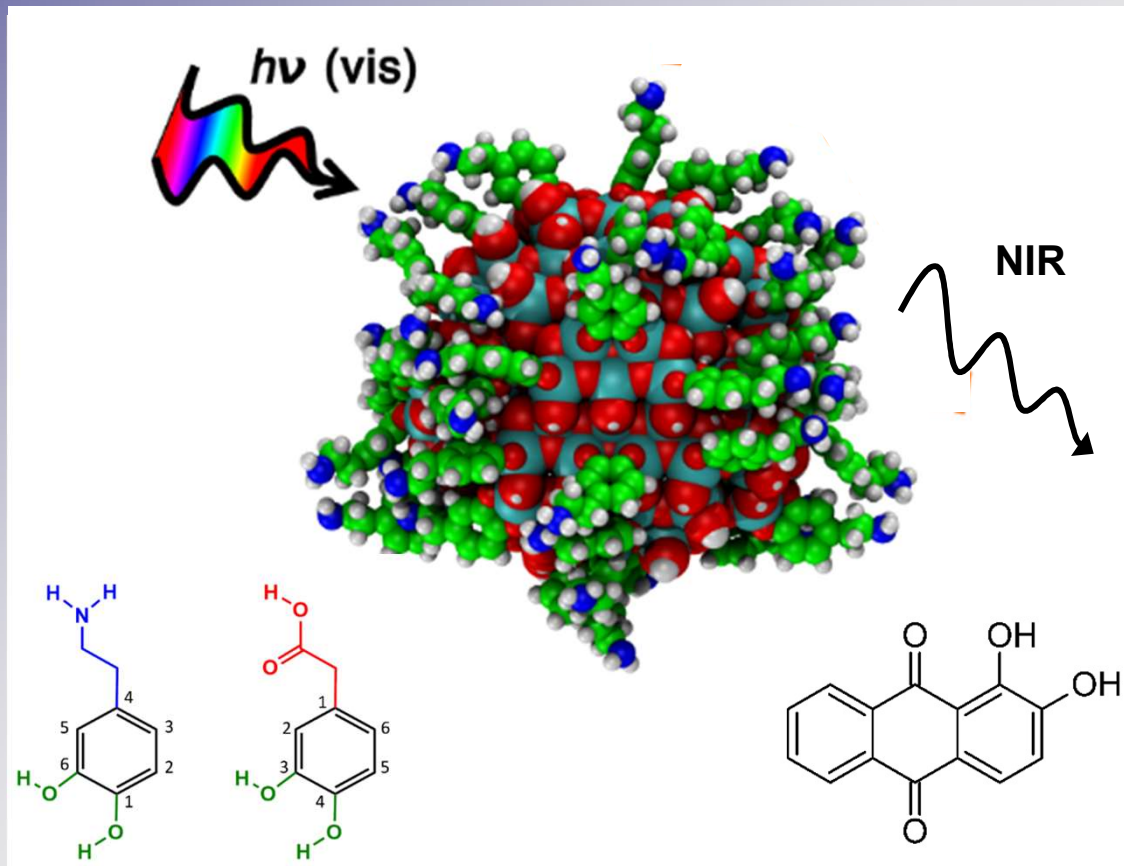


## MOLECULAR DYNAMICS AT 300 K

**15 PEG<sub>500</sub>  
IN WATER  
~33000  
molecules**



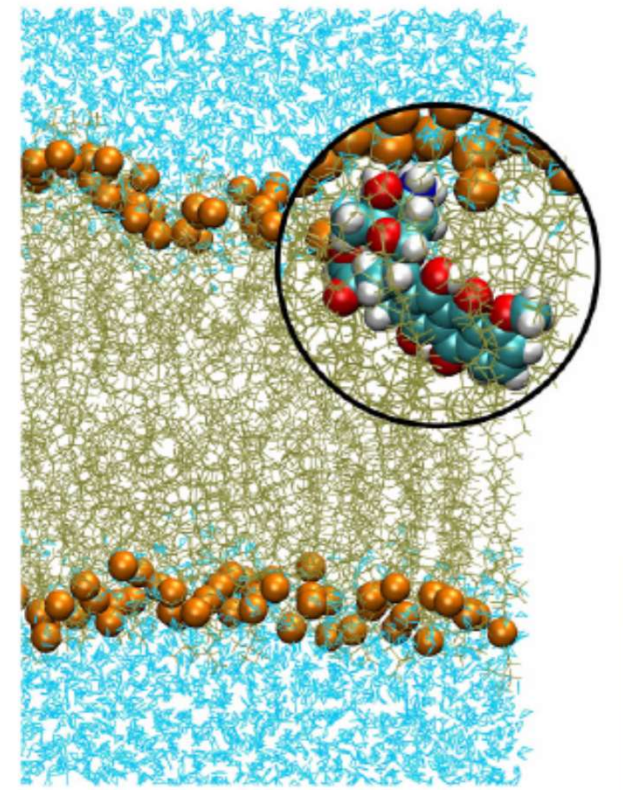
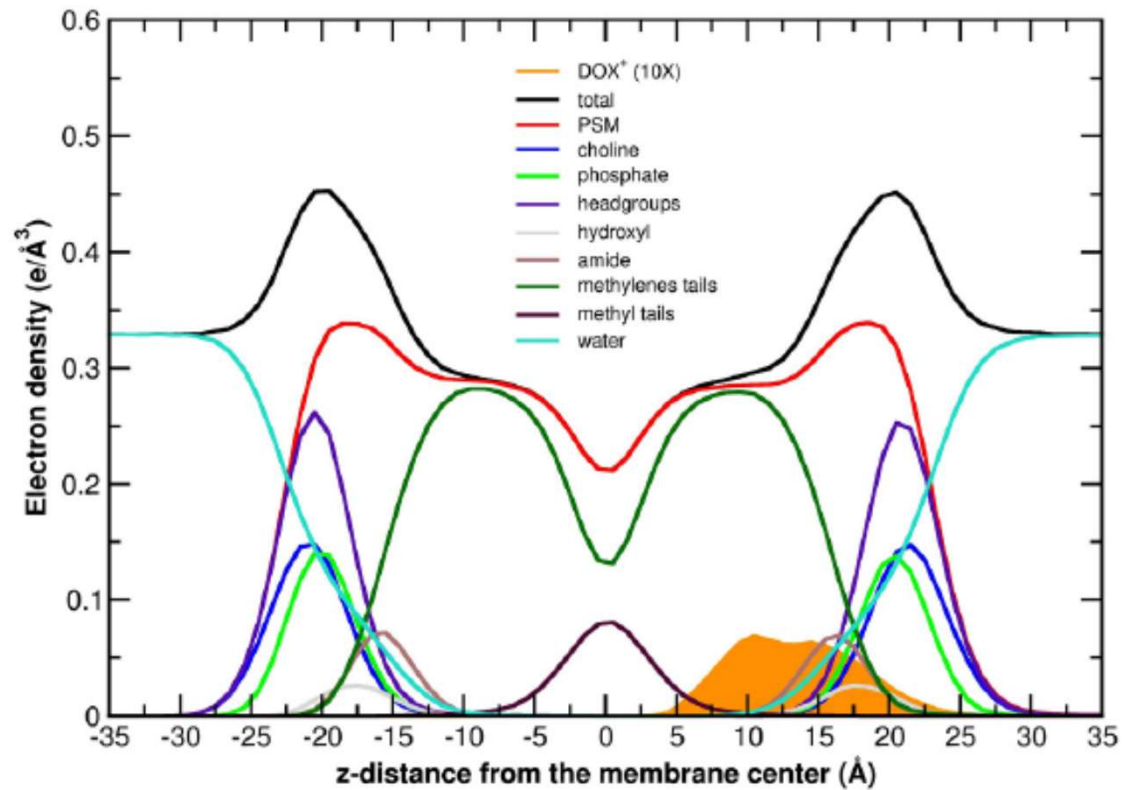
- TO MODIFY ABSORPTION REGION AND IMPROVE TISSUE PENETRATION FOR PHOTODYNAMIC THERAPY
- TO ACTIVATE FLUORESCENT PROPERTIES FOR IMAGING



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

## ROLE OF LIPID COMPOSITION

## DRUG OR NP

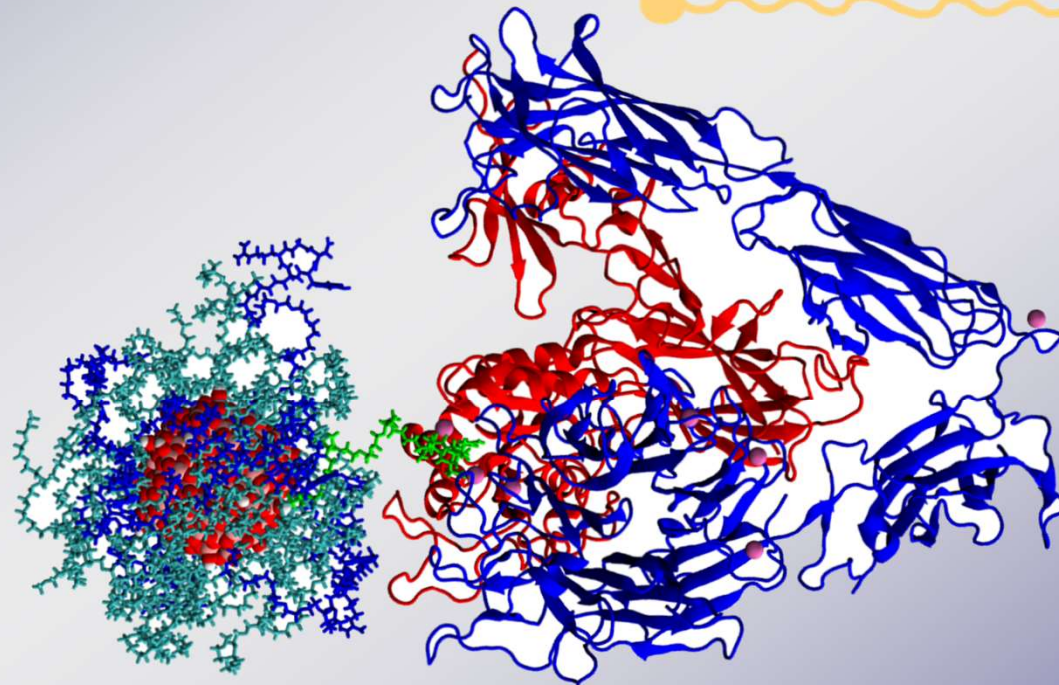
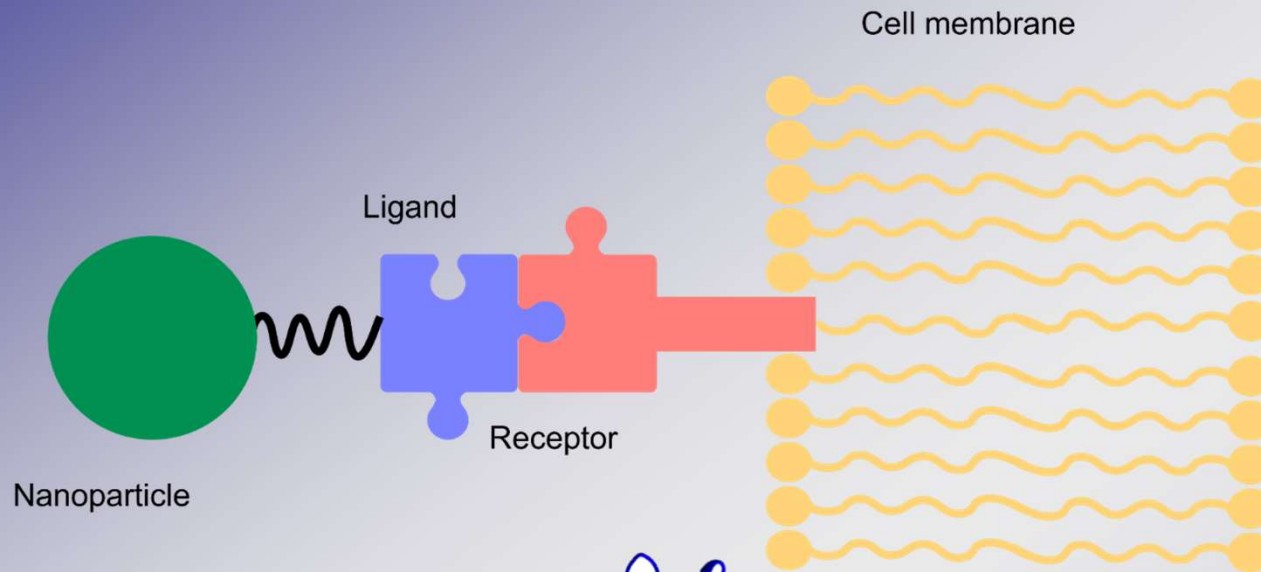


Siani, Donadoni, Ferraro, Re, CDV *BBA Biomembranes* **2022** 1864 183763

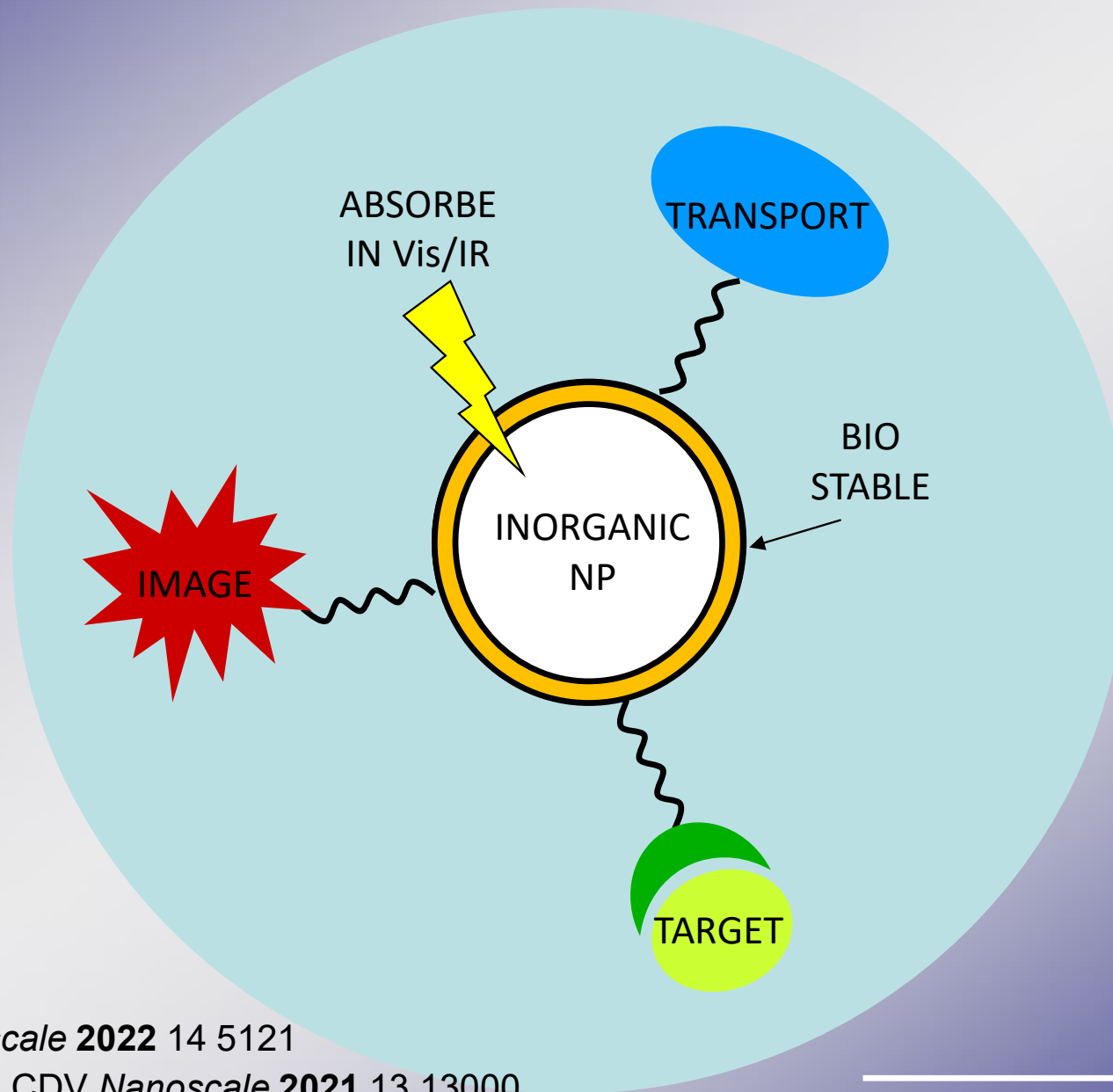
in collaboration with Prof. Francesca Re (Monza) &  
Prof. Qiang Cui (Boston)







STIMULI-RESPONSIVE NANOMATERIALS

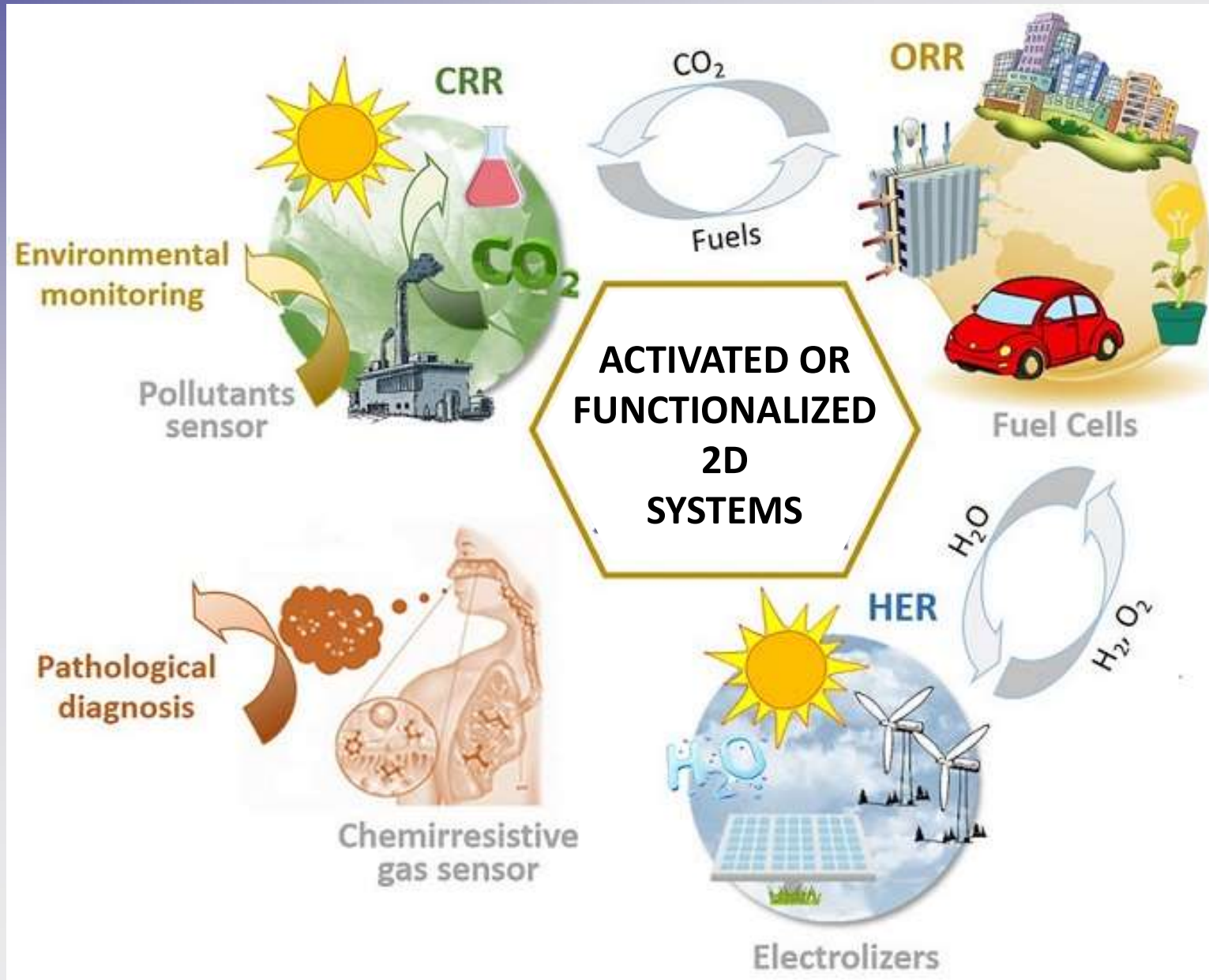


Siani, CDV *Nanoscale* **2022** 14 5121

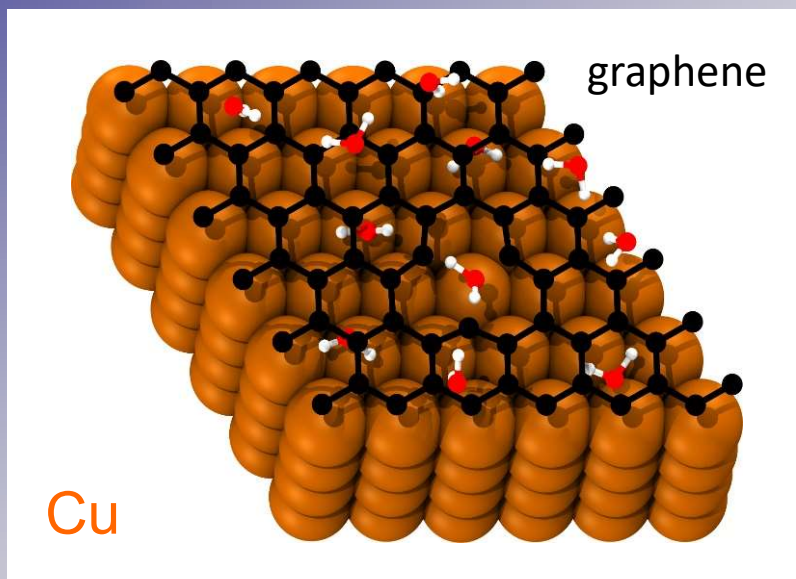
Motta, Siani, Levy, CDV *Nanoscale* **2021** 13 13000

Donadoni, Siani, Frigerio, CDV, *Nanoscale* **2022** 14 12099

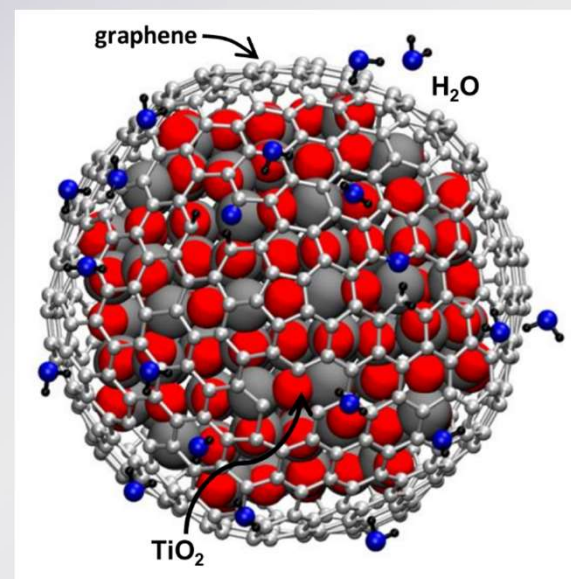
MILANO 16/01/2023



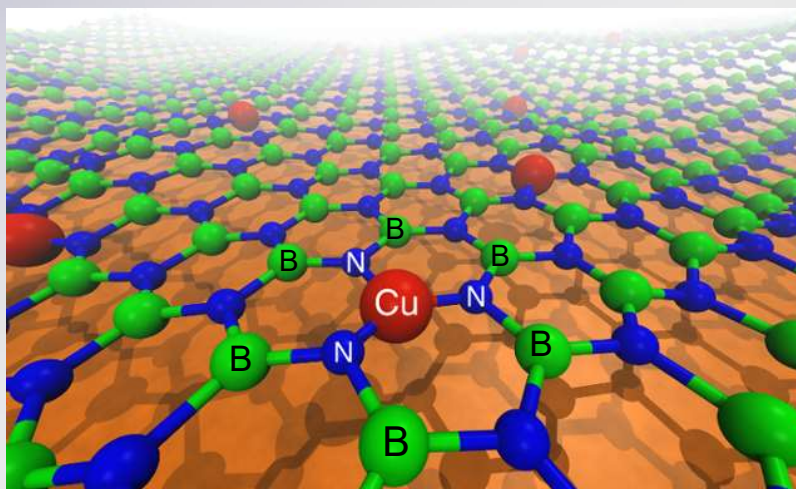




ACS AMI **2017** 9 29932



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



h-BN/Cu(111)

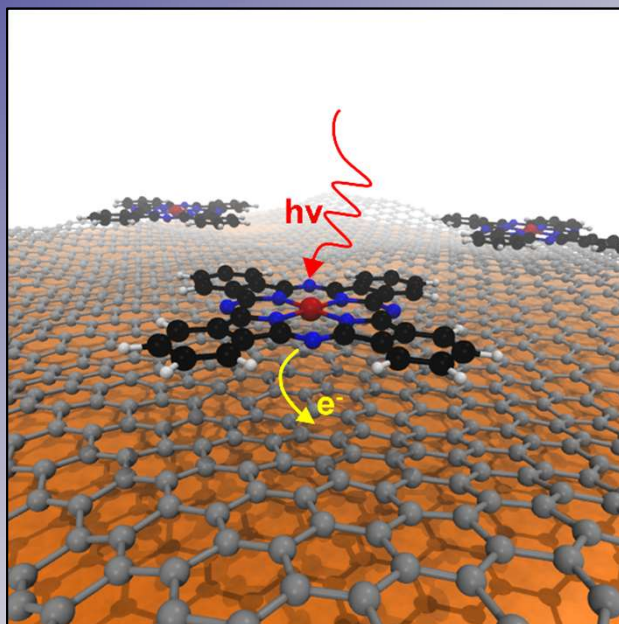
ChemSusChem **2019** 12 1995

CATALYSIS UNDER COVER

CATALYSIS BY  
METAL ATOMS TRAPPING

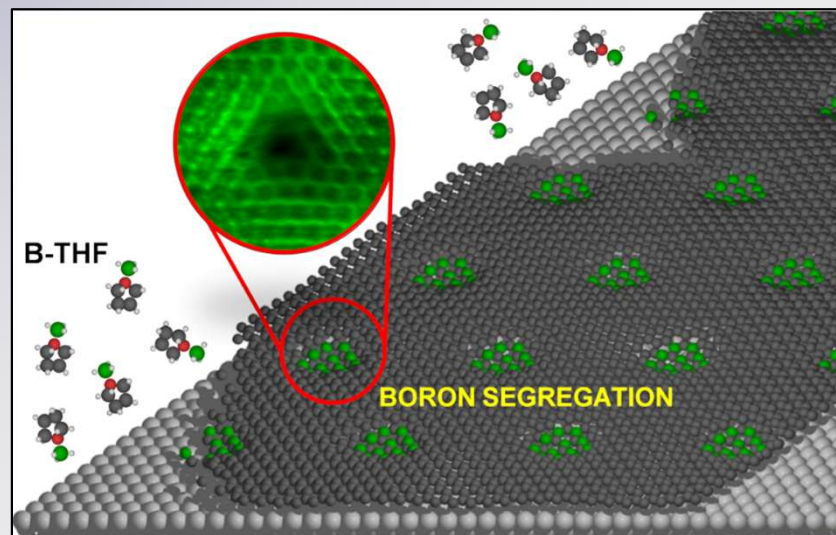
ELECTROCATALYSIS

## MOLECULAR INTERFACES



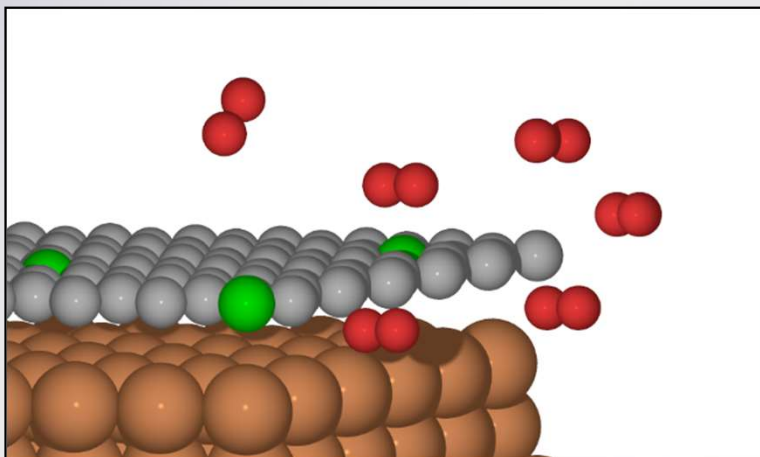
*ACS Nano* **2022** 16 10456

## DOPED GRAPHENE ON METAL SUBSTRATES

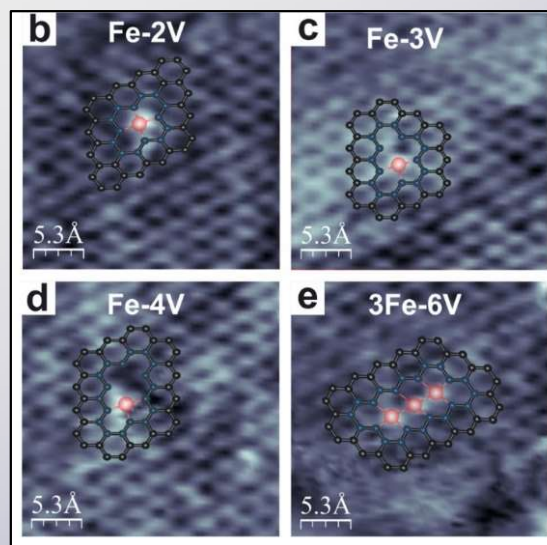


*Carbon* **2023** 201 881

## METAL INTERFACES

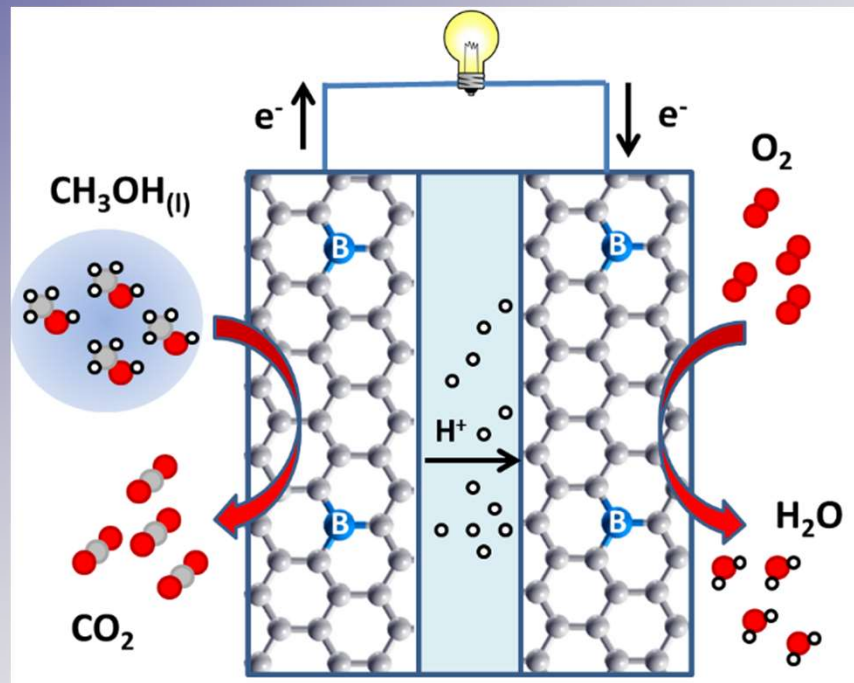


*J. Am. Chem. Soc.* **2016** 138 7365

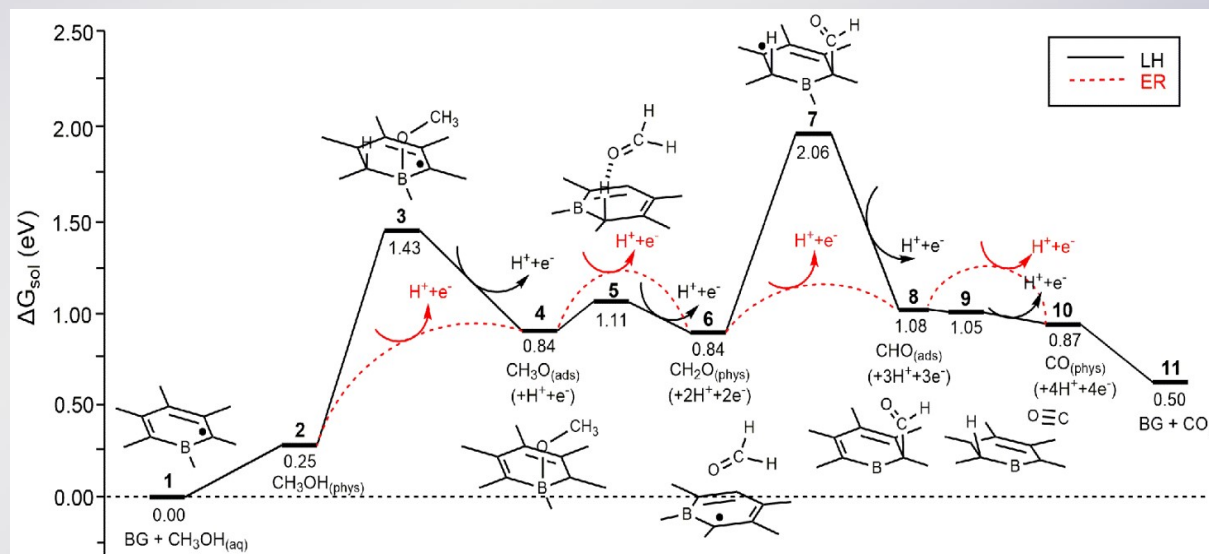


*Nature Catalysis* **2021** 4 850





**ELETTROCHIMICA  
COMPUTAZIONALE**







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 Department of Materials Science

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

Sincronizzazione non in corso

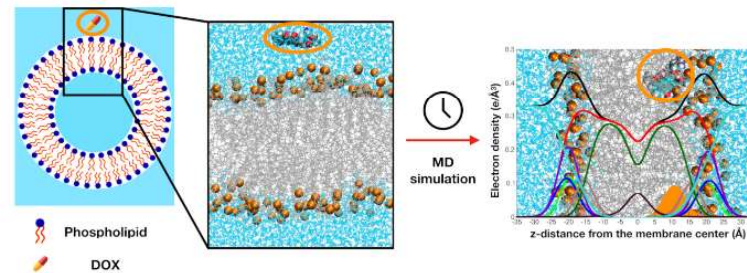
nanoQlab

Home Research People Equipment Publications Collaborations Funding

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 been awarded by CECAM for the best poster with...

Grazioli Prize 2021

February 17 2022: PhD student Edoardo Donadoni has been awarded by the Istituto Lombardo...

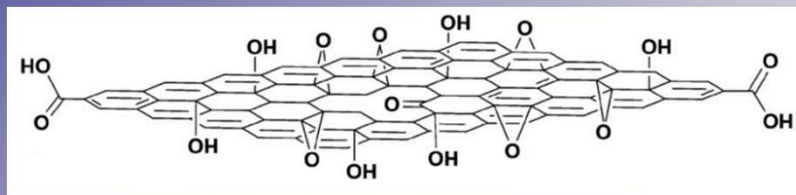
Master Exam

October 28 2021: Mirko Dolce received his Master's degree of finding the thesis 'Computational...

Windows taskbar with search bar and system tray

e-mail: cristiana.divalentin@unimib.it

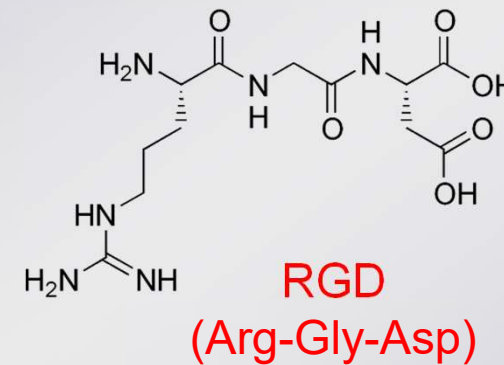
# GRAPHENE OXIDE



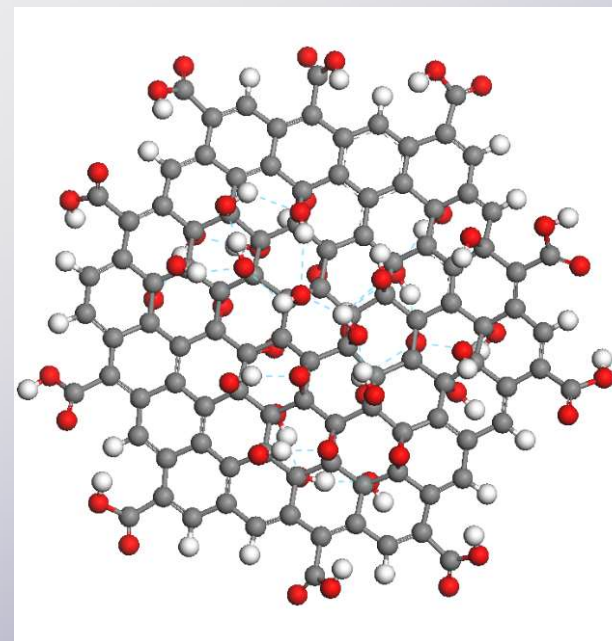
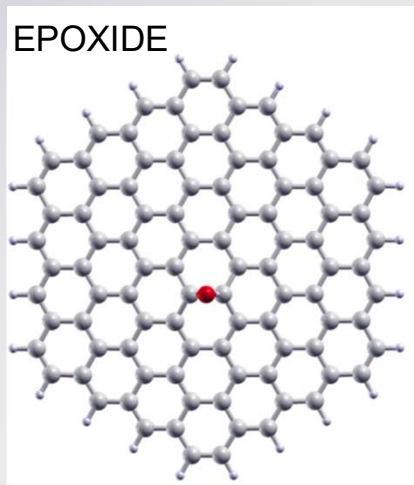
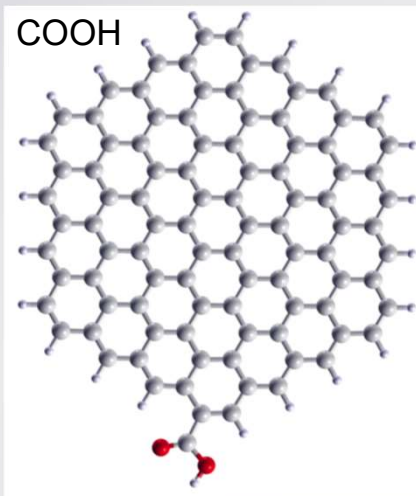
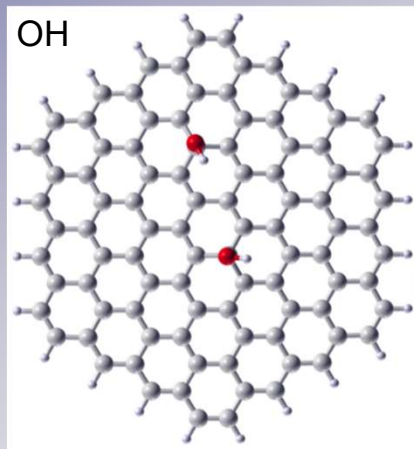
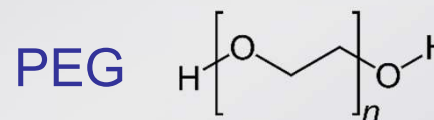
+

AMINOACIDS

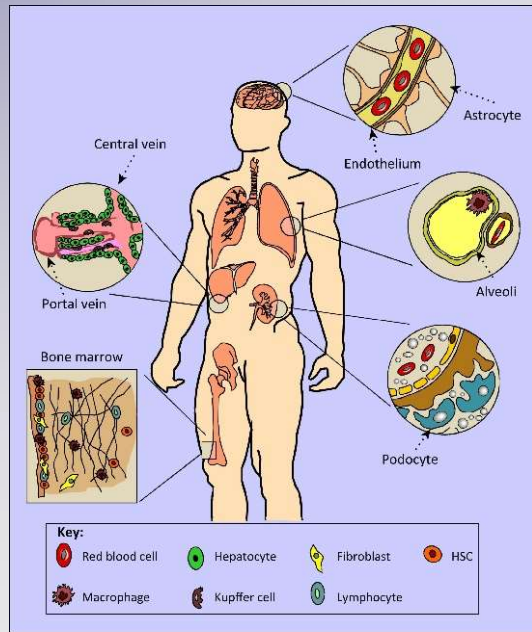
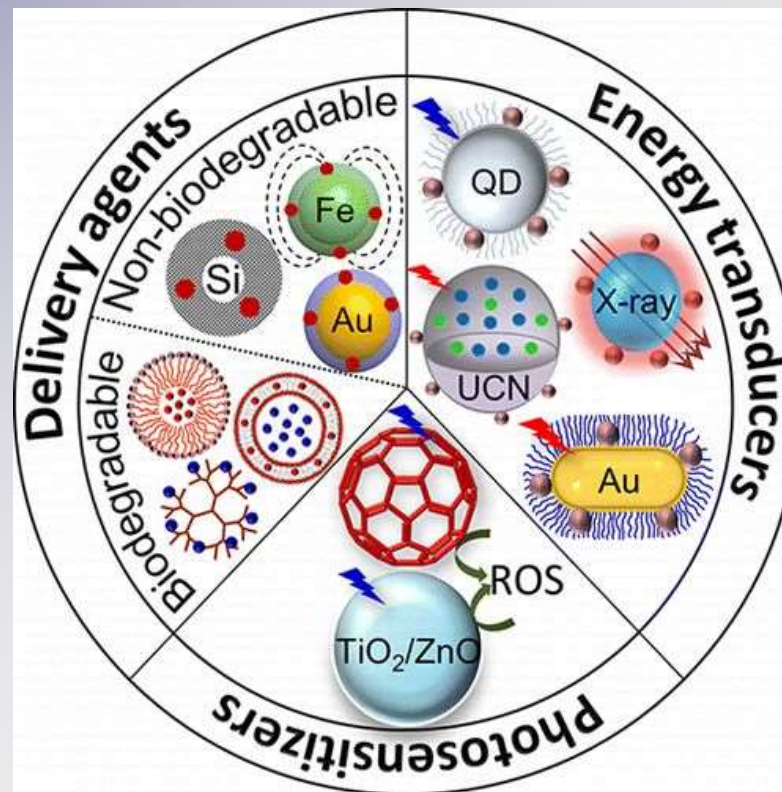
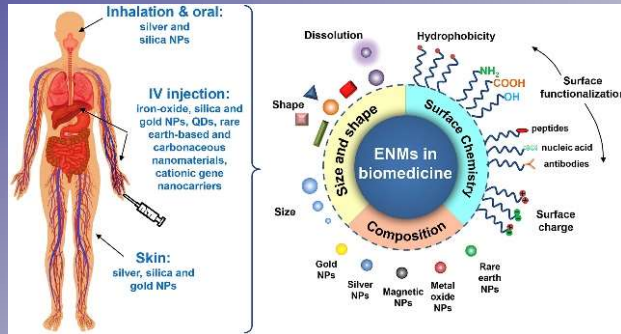
OLIGOPEPTIDES



**RGD**  
(Arg-Gly-Asp)







Trends in Biotechnology

