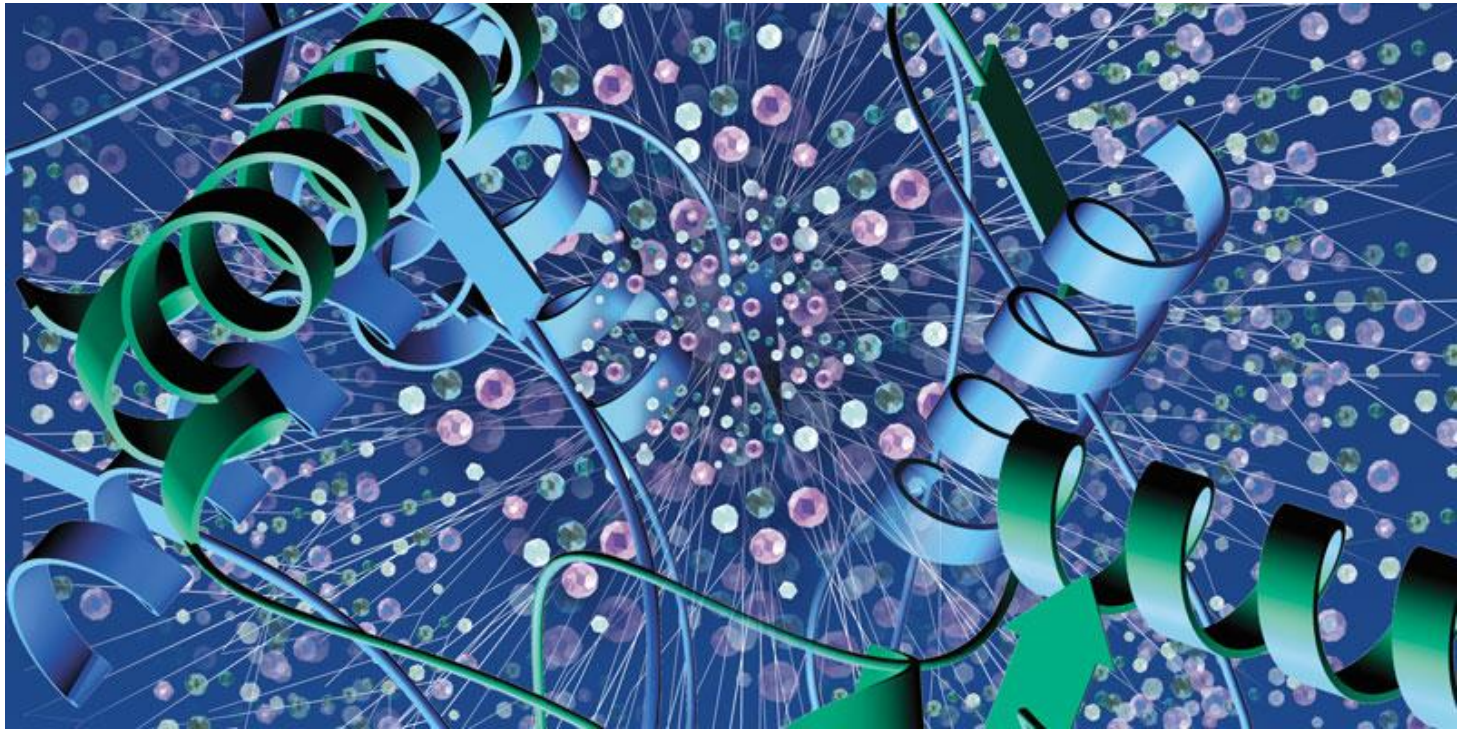
Biomolecole per lo sviluppo di materiali intelligenti



Giornate di orientamento per le tesi, Corso di Laurea in Fisica, 05/04/2024

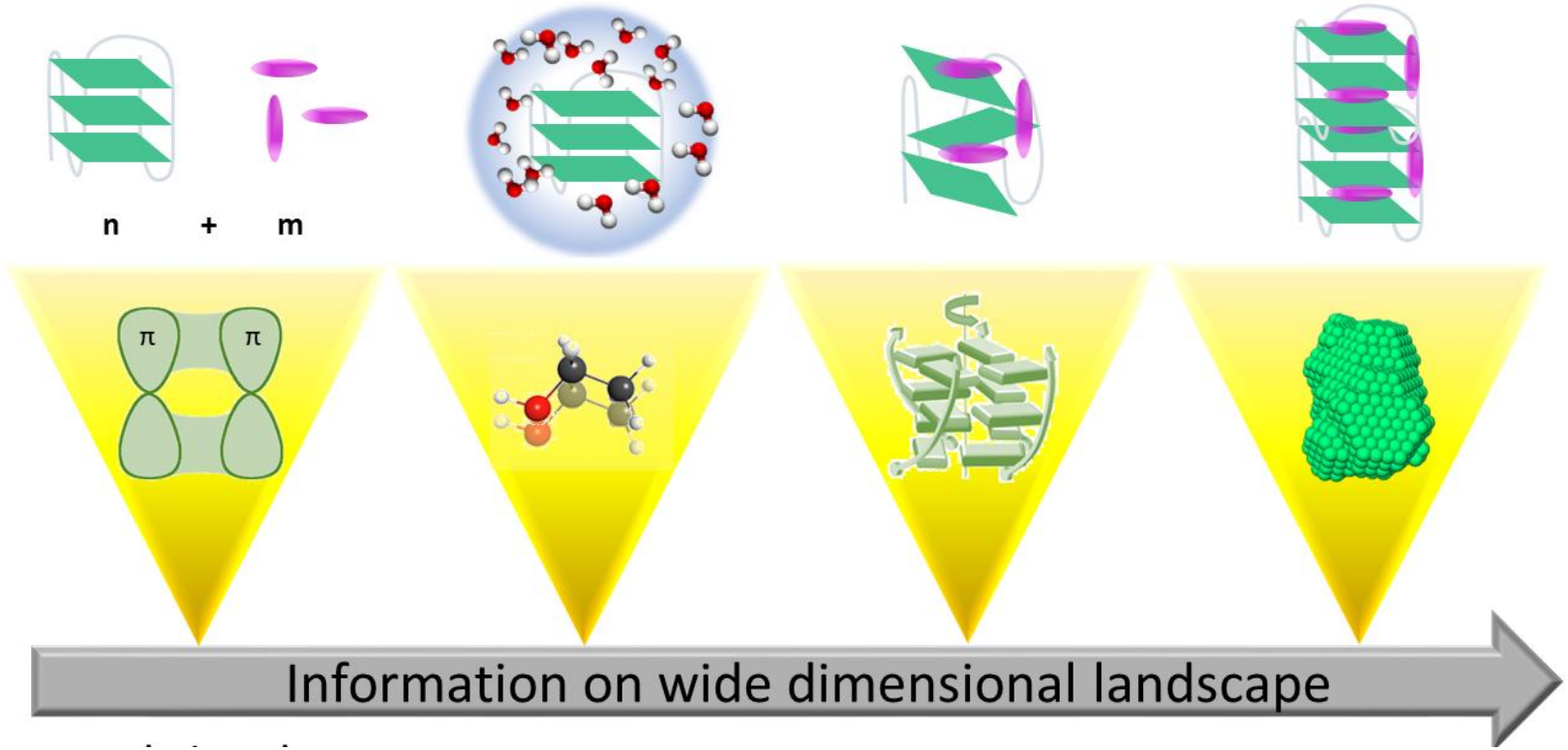
alessandro.paciaroni@unipg.it
valeria.libera@unipg.it
sara.catalini@unipg.it

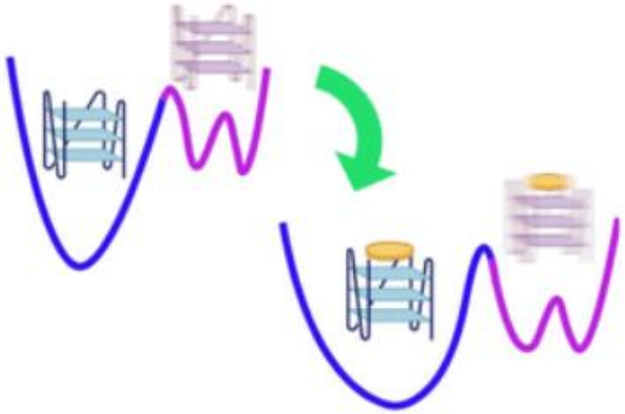
Cosa studiamo ?

Struttura

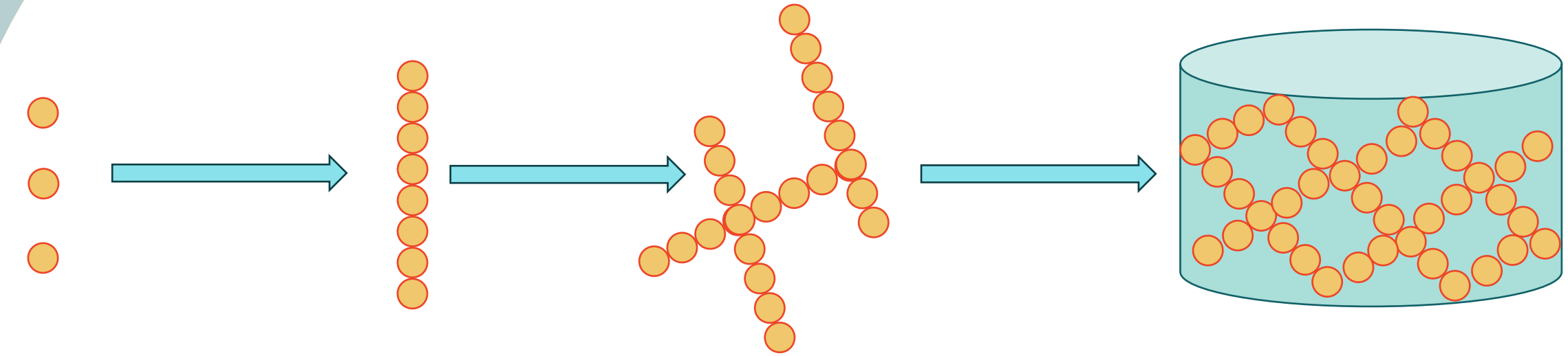
Interazione

Dinamica





Aggregazione gerarchica delle biomolecole: dal monomero al network polimerico



Monomero

Polimero

Aggregato Polimerico

Network Polimerico

Appel, E.A., et al., Chemical Society Reviews. 2012

Nano-aggregati e idrogel: applicazioni

Agricoltura

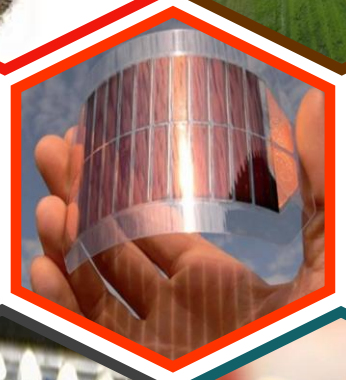
W.E. Rudzinski et al., Des. Monomers Pol. 2002

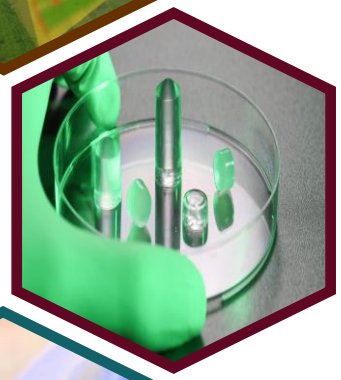
Industria Alimentare

X. Zhu et al., J. Adv. Res. 2022

Fotovoltaico

E. Meneghin et al., J. Phys. Chem. Lett. 2020



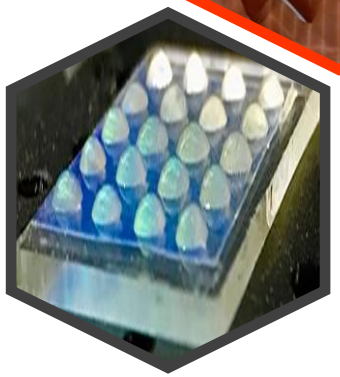


Trasporto dei farmaci

N.A. Peppas et al., Eur. J. Pharm. Biopharm. 2000

Biosensori

Y.S. Zhang et al., Science 2017



Ingegneria Tissutale

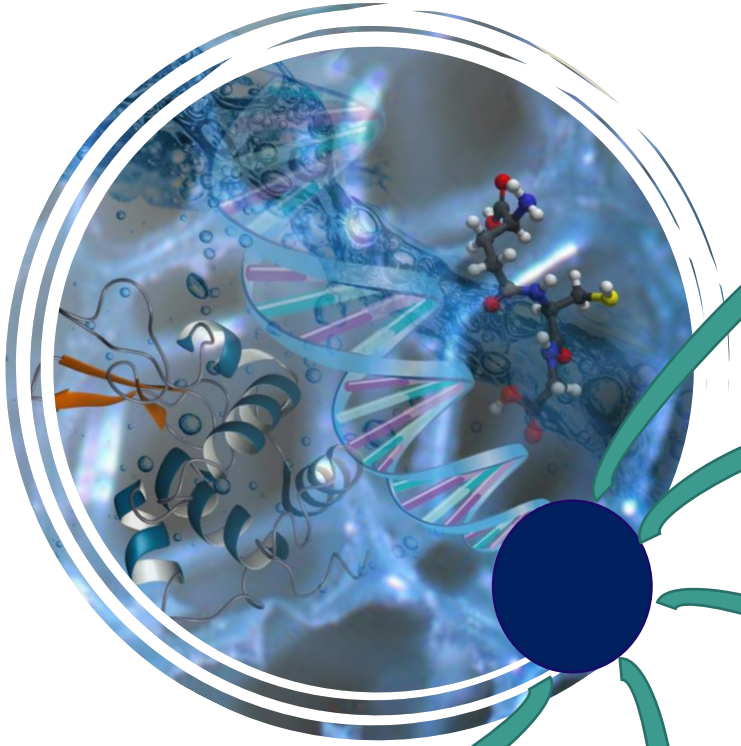
Q. Zou et al., J. Am. Chem. Soc. 2017

Medicina rigenerativa

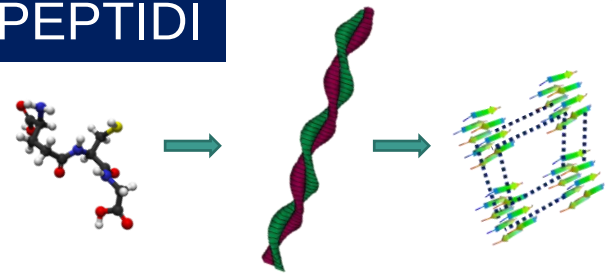
B.V. Slaughter et al., Adv. Mater. 2009

Scaffold cellulari

Sistemi intelligenti bio-inspirati

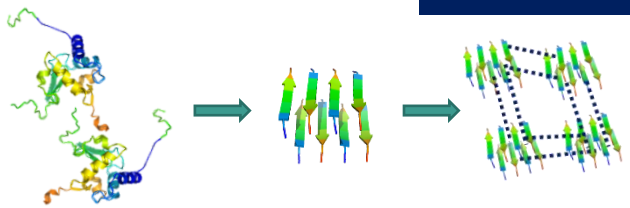


❑ PEPTIDI



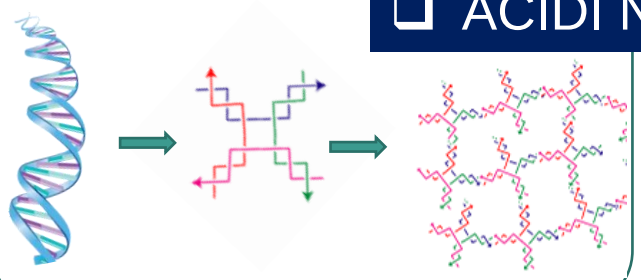
Marchesan, S., et al., **2014**. *Nanoscale*, *6*(10), pp.5172-5180.

❑ PROTEINE



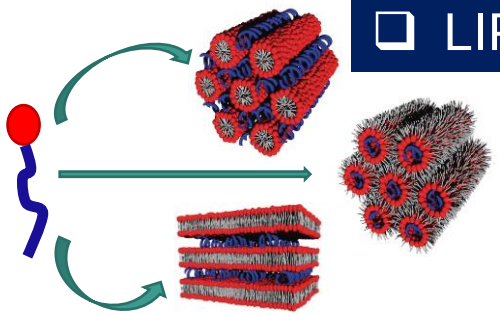
Cremades, N. and Dobson, C.M., **2018**. *Neurobiology of disease*, *109*, pp.178-190.

❑ ACIDI NUCLEICI



Lattuada, E., et al., **2020**. *Frontiers in Pharmacology*, *11*, p.1345.

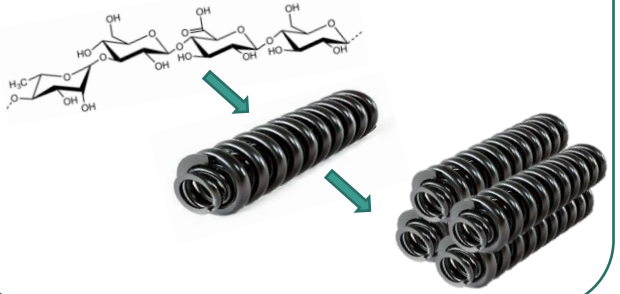
❑ LIPIDI



Sagalowicz, L., et al., **2006**. *Trends in Food Science & Technology*, *17*(5), pp.204-214.

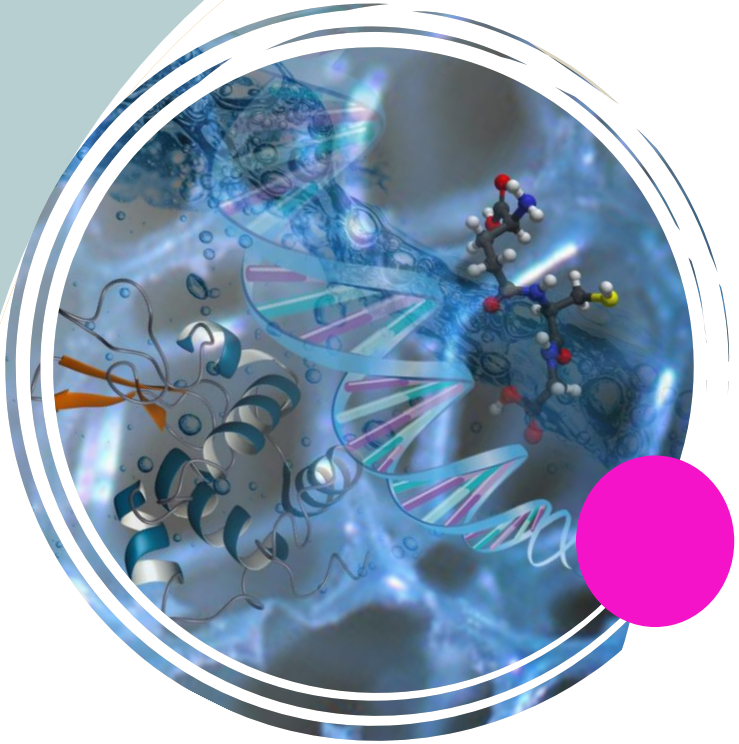
Diener, M., et al., **2020**.
ACS Macro Letters, *9(1), pp.115-121*

❑ CARBOIDRATI

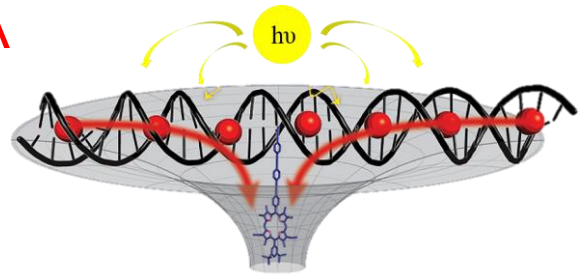


Sistemi fotosintetici bio-inspirati

Sfruttando la capacità delle **biomolecole** di **auto-aggregare** vogliamo riprodurre artificialmente dei sistemi in grado di **trasferire energia**, prendendo ispirazione dai complessi proteici fotosintetici.

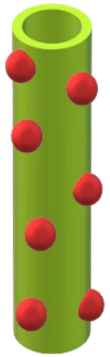


DNA



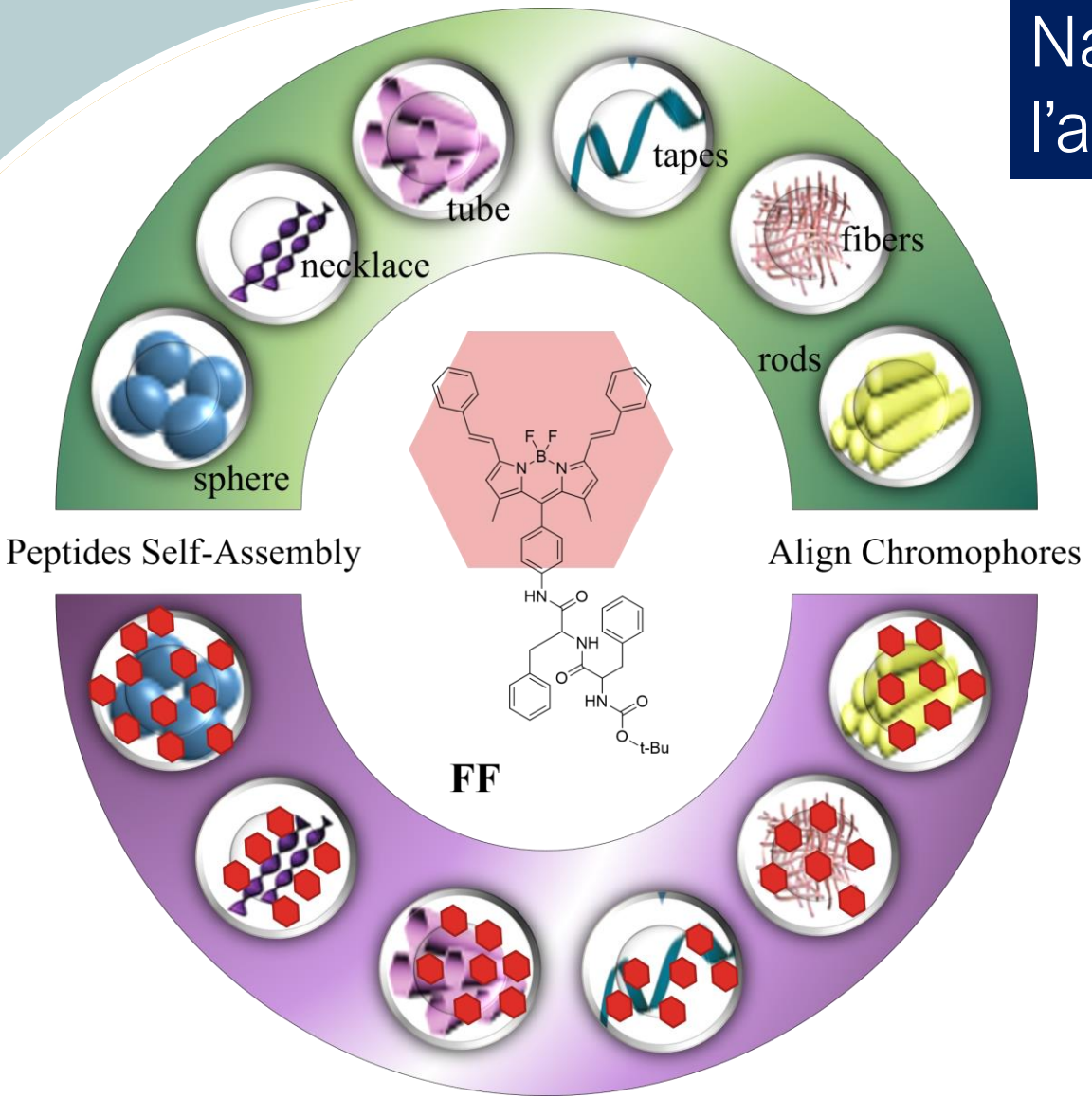
J.G. Woller et al., J. Am. Chem. Soc. 2013

PEPTIDI

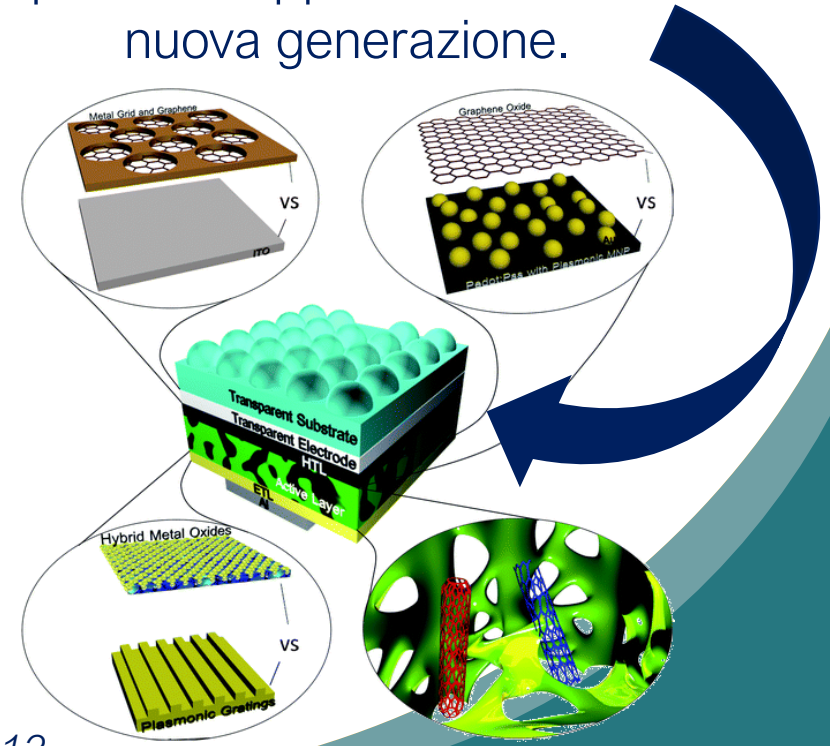


Q. Zou et al., Adv. Mater. 2016

Nano-aggregati formati attraverso l'auto-aggregazione di peptidi corti



Attraverso il controllo della **struttura** e della **morfologia** degli aggregati peptidici si può controllare la **spaziatura** e l'**orientazione** tra i cromofori, entrambi sono parametri essenziali per avere il **trasferimento di energia**.
Lo scopo è quello di produrre degli **strati attivi** efficienti per lo sviluppo di **celle solari ibride** di nuova generazione.

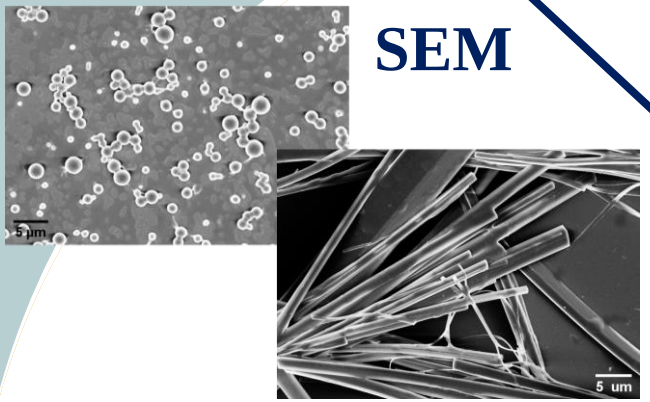


Jayawardena, K.I., et al. Nanoscale. 2013

approccio multitecnica

MORFOLOGIA

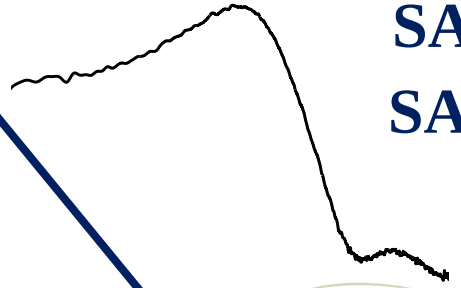
SEM

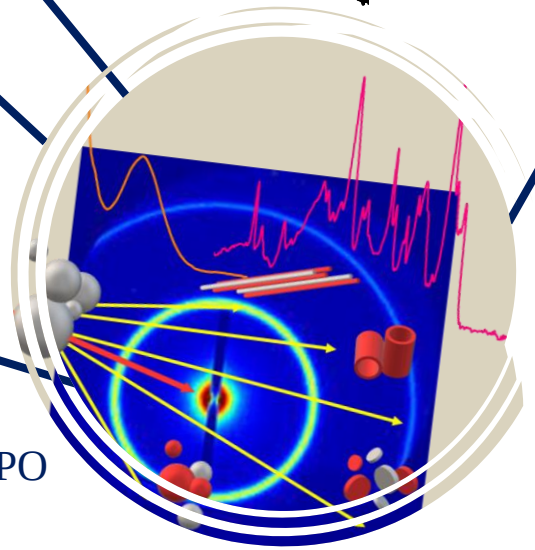


STRUTTURA

SAXS

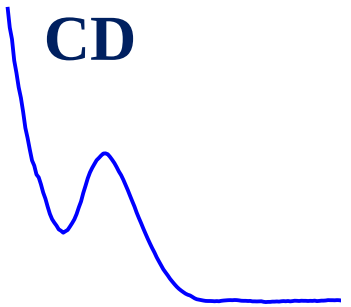
SANS





CONFORMAZIONE

CD

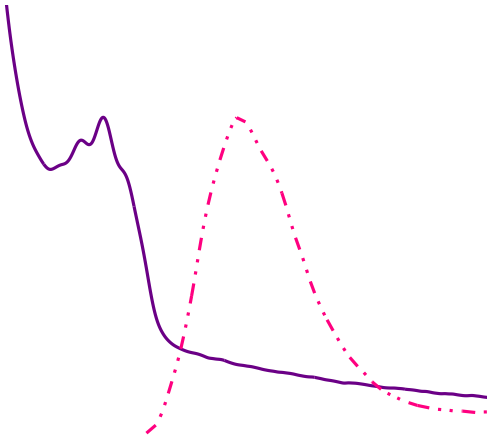


ATR-IR

PROPRIETÀ FOTOFISICHE

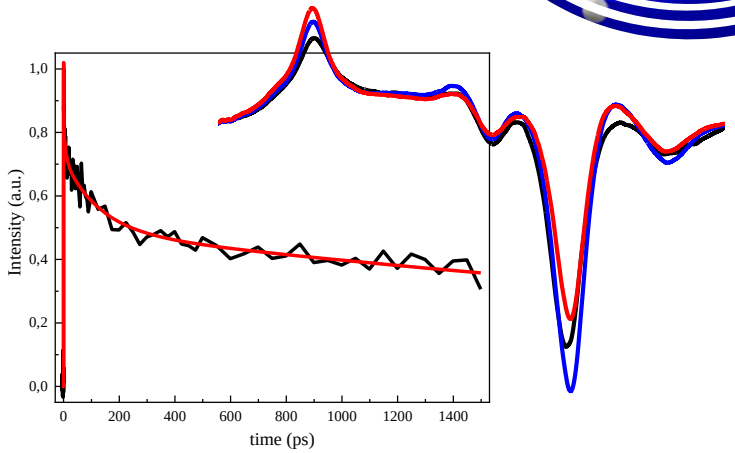
ABS. & FLUO.

STAZIONARIE



TAS

RISOLTE IN TEMPO



PROGETTO VITALITY

VITALITY

2023-2025: **PRIN** 2022 project *Efficient Light Harvesting with Self-assembled Peptide Nanostructures (*LANTERN*)*

Materials Advances

ROYAL SOCIETY OF CHEMISTRY

PAPER

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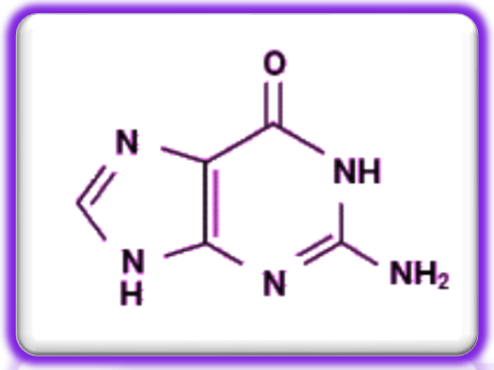
Cite this: DOI: 10.1039/d4ma00018h

Multiple length-scale control of Boc-protected diphenylalanine aggregates through solvent composition†

Sara Catalini,[abc] Francesco Bagni,[cd] Stefano Cicchi,[d] Mariangela Di Donato,[ce] Alessandro Iagatti,[bc] Andrea Lapini,[cf] Paolo Foggi,[bcg] Caterina Petrillo,[a] Alessandro Di Michele,[a] Marco Paolantoni,[g] Giorgio Schirò,[h] Lucia Comez[*i] and Alessandro Paciaroni[*a]

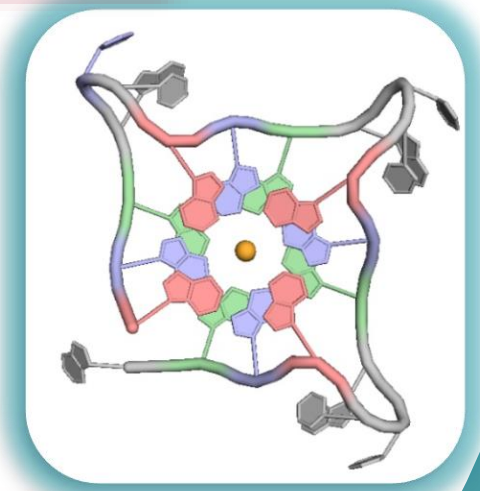
DNA non canonico

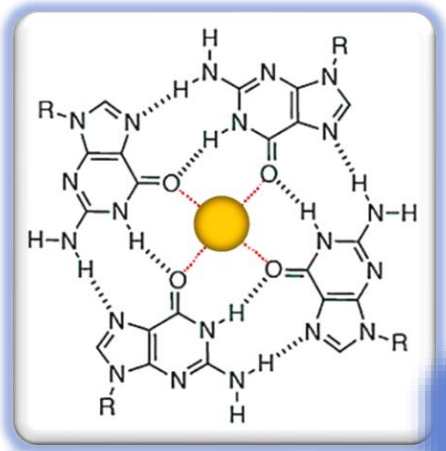
Catione monovalente



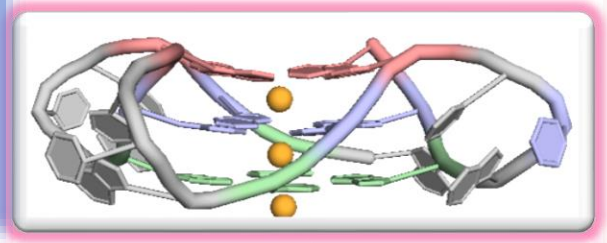
Guanine

G-quadruplex





Legame idrogeno Hoogsteen

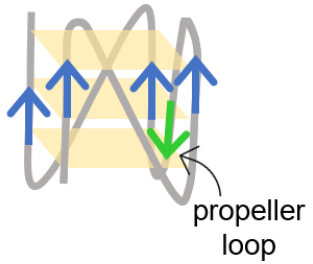


Interazione di stacking tra le guanine delle tetradi

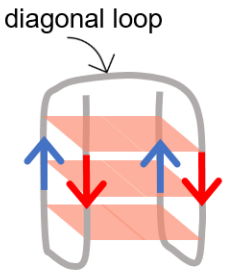
Strutture secondarie di G-quadruplex

Topologie di G4

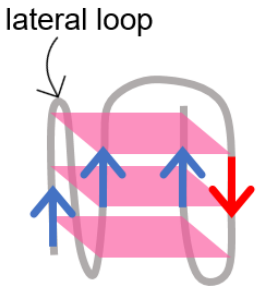
- **Parallela**



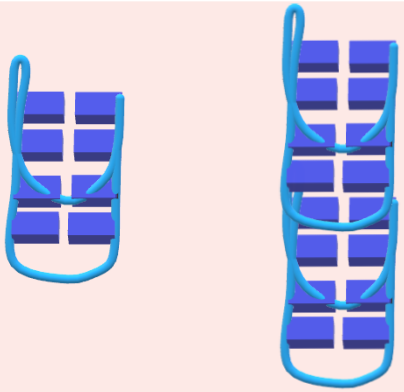
- **Antiparallela**



- **Ibrida**



- **Multimeri**



La struttura e la stabilità dei G4 dipende da vari fattori: sequenza, lunghezza dei loop, concentrazione e tipi di cationi.

PROGETTO VITALITY

2023-2025: **PRIN** 2022 project *Taming Structure, Conformation and Stability of Multimeric G-quadruplex DNA (***TAMeQUAD***)*

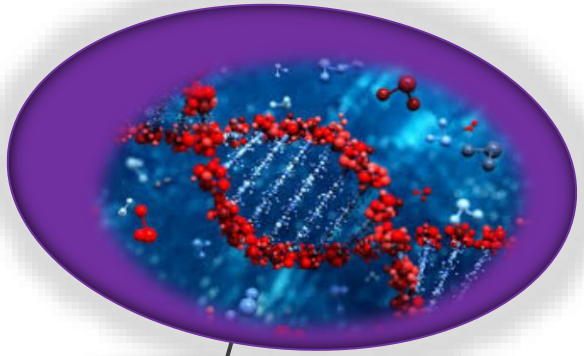
J|A|C|S JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

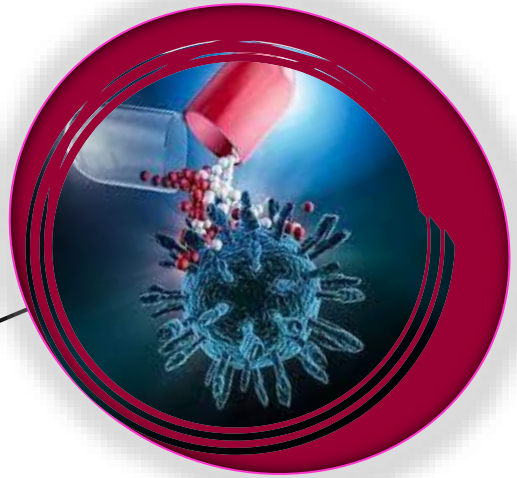
pubs.acs.org/JACS Article

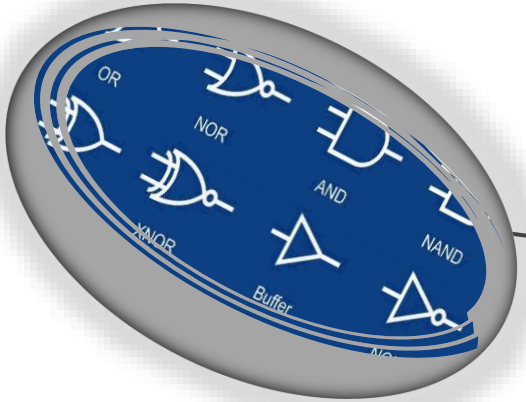
Stacking Interactions and Flexibility of Human Telomeric Multimers

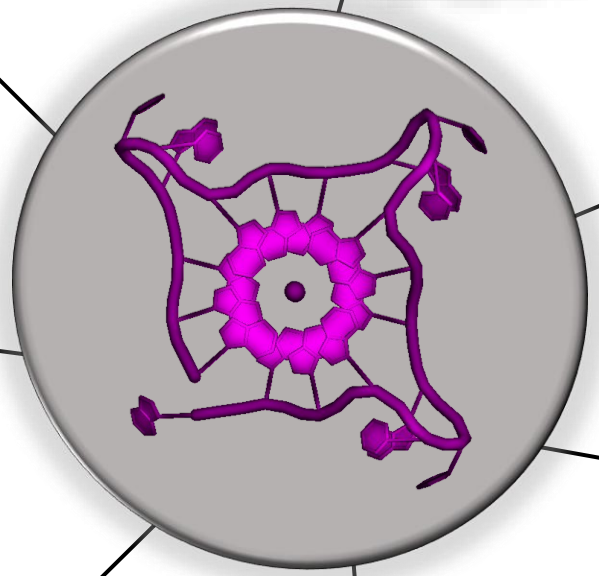
Benedetta Petra Rosi, Valeria Libera, Luca Bertini, Andrea Orecchini, Silvia Corezzi, Giorgio Schirò, Petra Pernot, Ralf Biehl, Caterina Petrillo, Lucia Comez,*,○ Cristiano De Michele,*,○ and Alessandro Paciaroni*,○

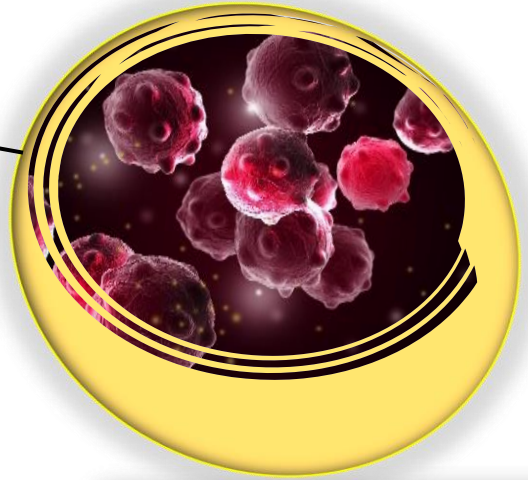
Cite This: *J. Am. Chem. Soc.* 2023, 145, 16166−16175 Read Online

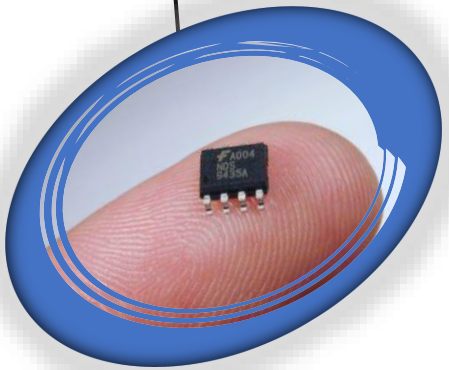












Applicazioni

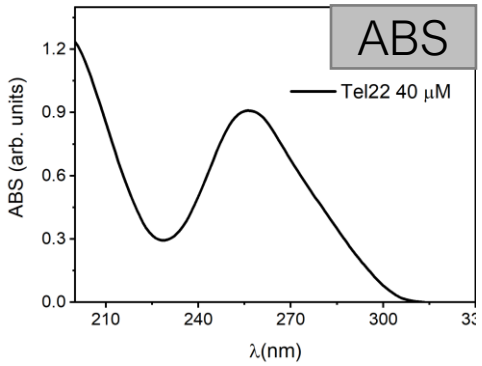
Come? Dove?

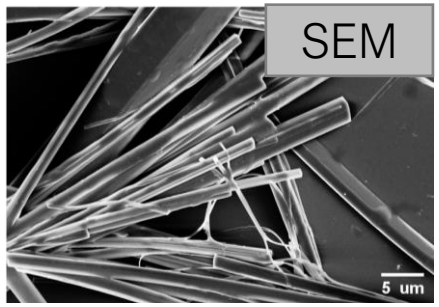
In-house

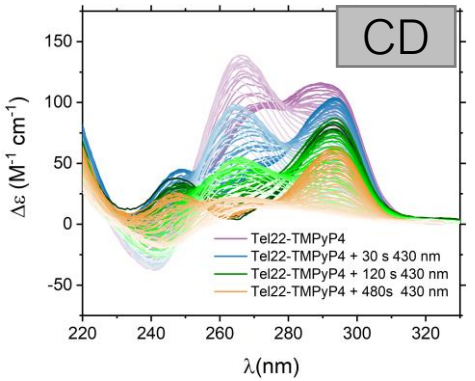
- Preparazione campioni
- Spettroscopia di assorbimento UV-visible (ABS)
- Microscopia a scanzione elettronica (SEM)
- Dicroismo circolare (CD)
- Spettroscopia di fluorescenza (Fluo)
- Spettroscopia infrarossa (IR)

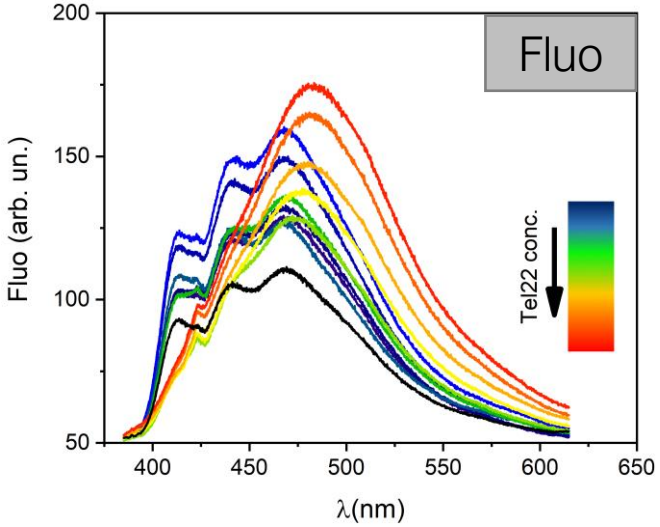
Preparazione del campione

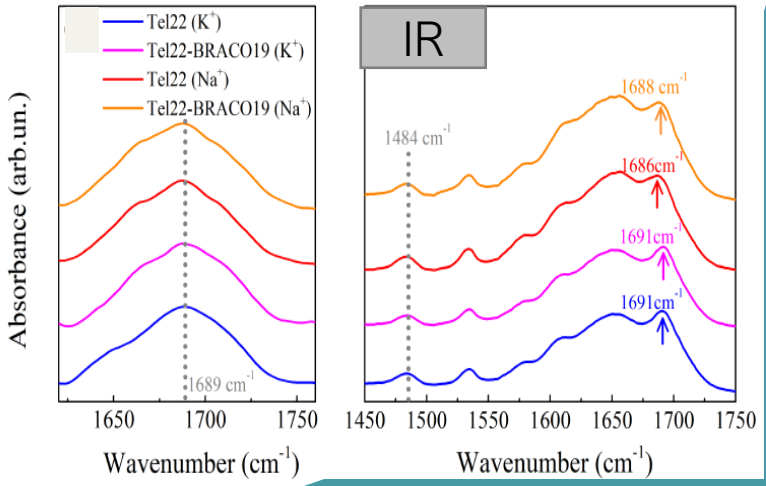
Tecniche di indagine







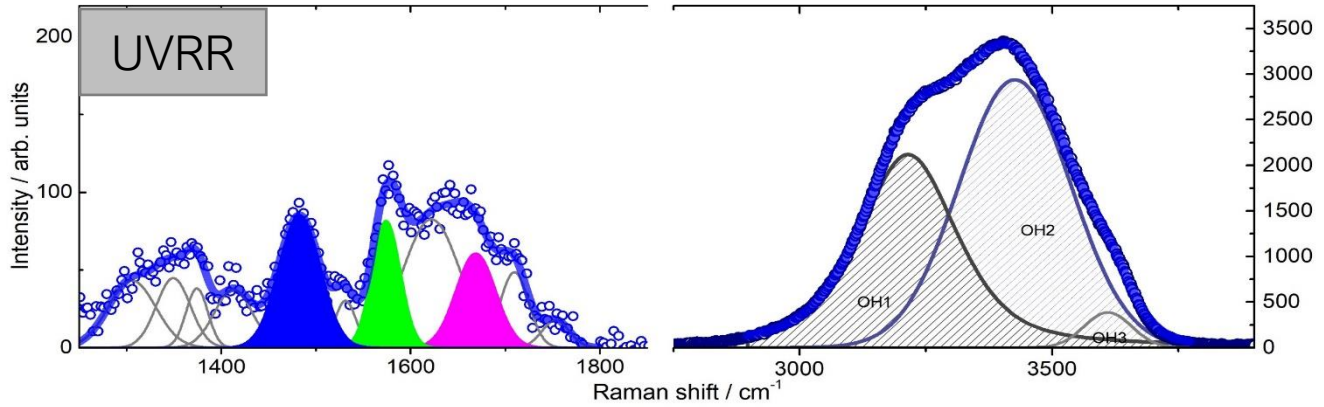


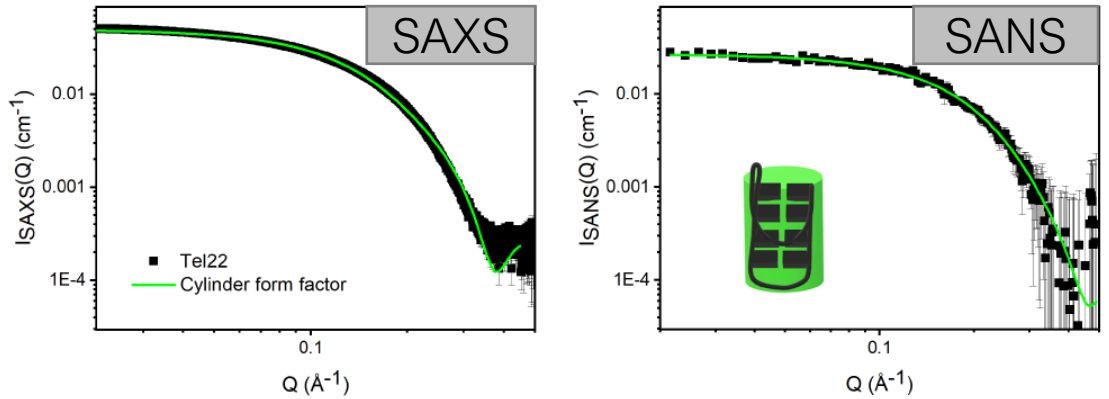


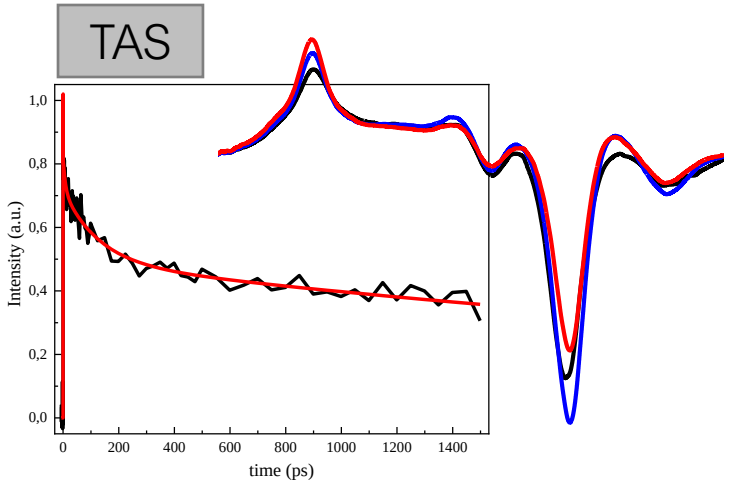
Come? Dove?

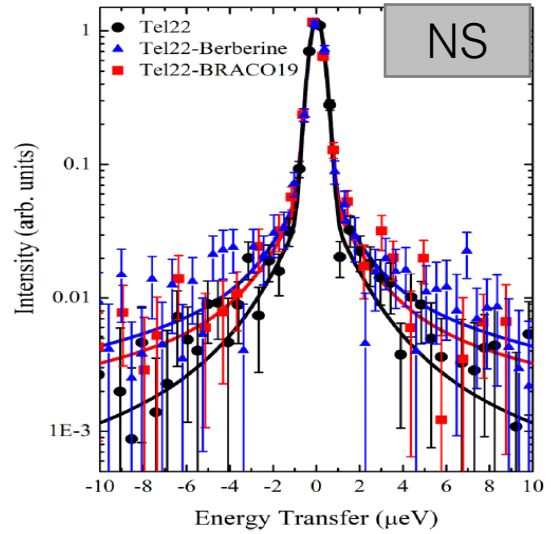
Large scale facilities

- UV-Raman Risonante (UVRR) (Elettra synchrotron Trieste)
- Scattering di raggi X a basso angolo (SAXS) (ESRF synchrotron Grenoble)
- Scattering di neutroni a basso angolo (SANS) (ILL Grenoble)
- Spettroscopia di assorbimento transiente (TAS) (LENS Firenze)
- Scattering di neutroni (NS) (ILL Grenoble)



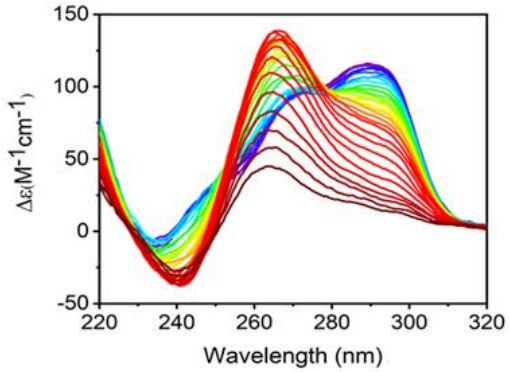




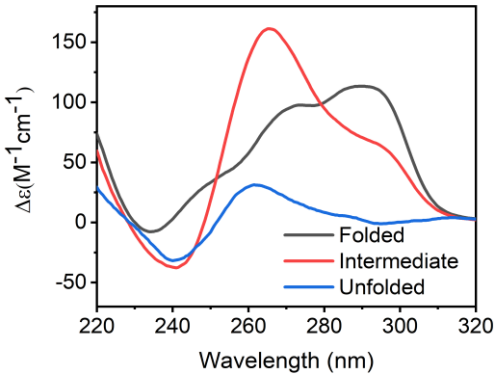


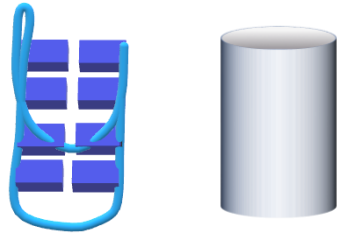
Come?

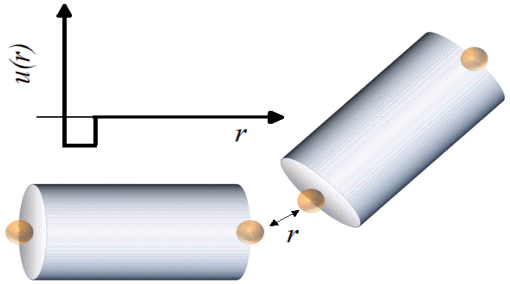
- Analisi multivariata
- Sviluppo di nuovi programmi per la modellizzazione del sistema
- Simulazioni extremely coarse-grained (ECGS)



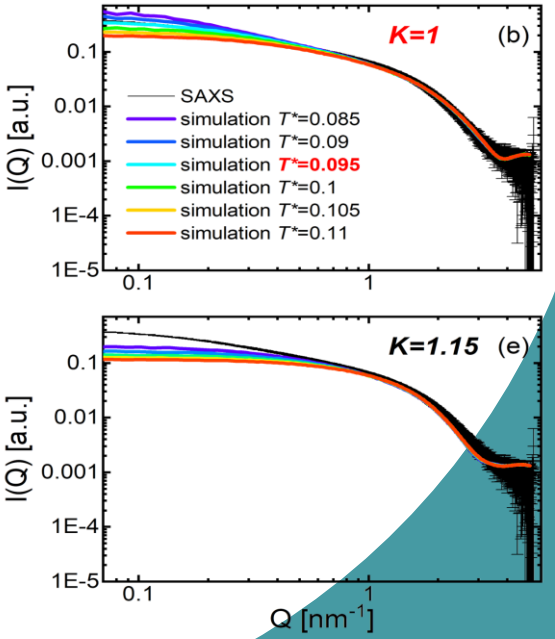
SVD







ECGS



Proposte tesi

Tesi triennali

- ✓ Analisi termodinamica del melting del G-quadruplex e dell'effetto di stabilizzazione derivato dall'interazione con farmaci antitumorali.
- ✓ Studio cinetico e strutturale del processo di aggregazione di peptidi corti.

Tesi magistrali

- ✓ Studio di processi d'interazione tra G-quadruplex e ligandi fotosensibili per lo sviluppo di nano-materiali intelligenti.
- ✓ Descrizione di processi di multimerizzazione del G-quadruplex.
- ✓ Sviluppo di programmi per l'analisi dei dati di scattering a basso angolo.
- ✓ Studio dell'aggregazione di peptidi corti decorati con cromofori per applicazioni fotovoltaiche e fototerapiche.

Chi?

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- Dr. Lucia Comez
- Prof. Caterina Petrillo
- Prof. Andrea Orecchini

- Dr. Sara Catalini
- Dr. Valeria Libera
- Luca Bertini (PhD)

- Mattia Trappella (PhD)
- Rocco Malaspina (PhD)
- Beatrice Caviglia (PhD)