



# Integrating Theory and Experiment: Ab Initio and Molecular Docking Approaches in Carbon Nanostructures

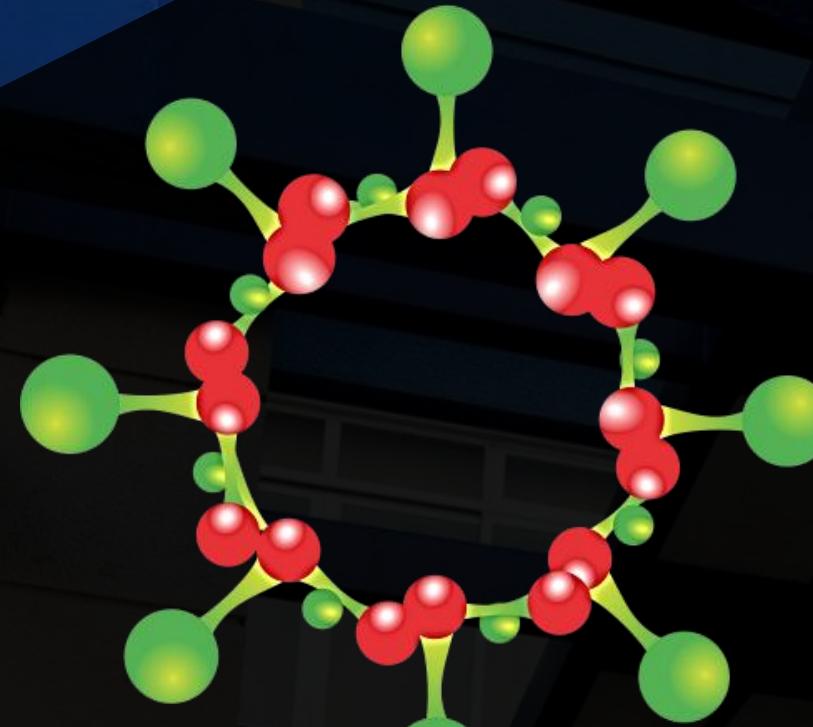
**Solange Binotto Fagan**  
Franciscan University - UFN  
Santa Maria – RS, Brazil



## Santa Maria



# NANOSCIENCE PROGRAM (MASTER and PhD)



Universidad



INTERNATIONAL IBERIAN  
NANOTECHNOLOGY  
LABORATORY



National Institute of Science and Technology  
Carbon Nanomaterials

## Lines of Research

- ▼ Development and characterization of Bioactive and Nanostructured Systems
  
- ▼ Modeling and Simulation of Biosystems and Nanomaterial



WASTEWATER  
TREATMENT

BIO  
REMEDIATION

BIO SENSORS

NANO  
ENVIRONMENT  
BIO

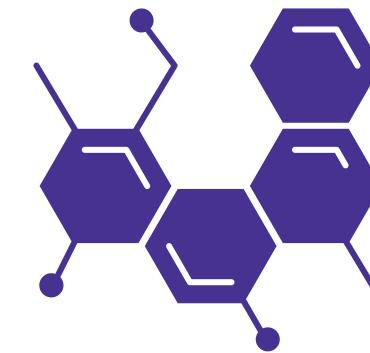
NANO  
TOXICITY

DRUG  
DELIVERY

NANO  
ADSORBENTS

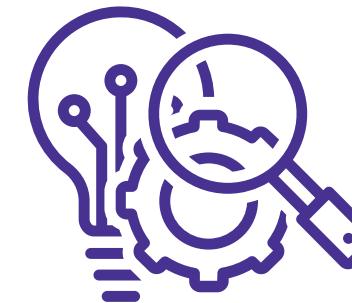


# SIMULATION/MODELING X EXPERIMENTAL CORRELATION



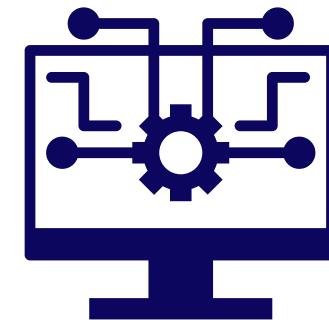
## NANOMATERIALS

- GRAPHENE AND DERIVATIVES
- NANOTUBES
- POLYMERS
- CYCLODEXTRINS
- ...



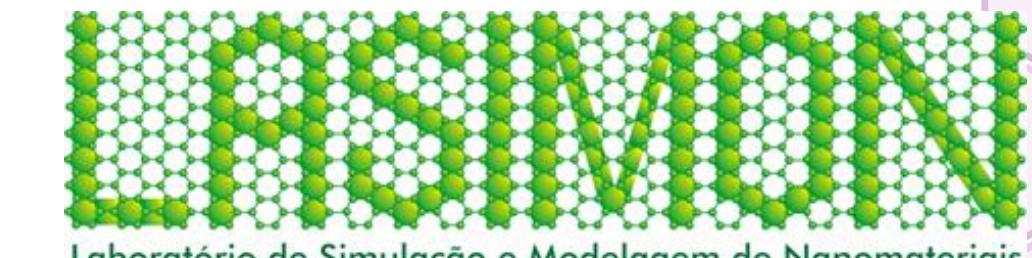
## EXPERIMENTAL ANALYSIS

- BIOLOGICAL OR CHEMICAL ADSORPTION
- BIOLOGICAL INTERACTION
- CHARGE TRANSFER
- ELECTRONIC/TRANSPORT BEHAVIOR
- THERMODYNAMIC CONDITIONS
- ...



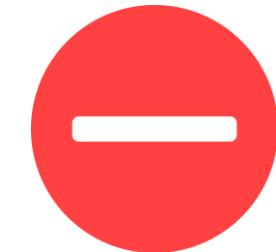
## METHODOLOGIES

- AB INITIO SIMULATIONS
- MOLECULAR DOCKING
- MOLECULAR DYNAMICS

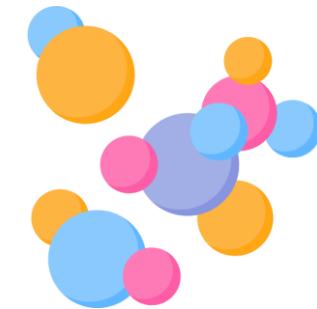


# *Ab Initio* simulations - Density Functional Theory (DFT)

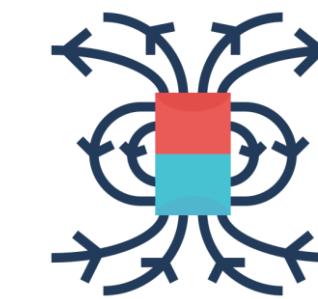
Describe many-body quantum systems to study their properties without dependence on empirical/experimental values



Electronics



Structural



Magnetic

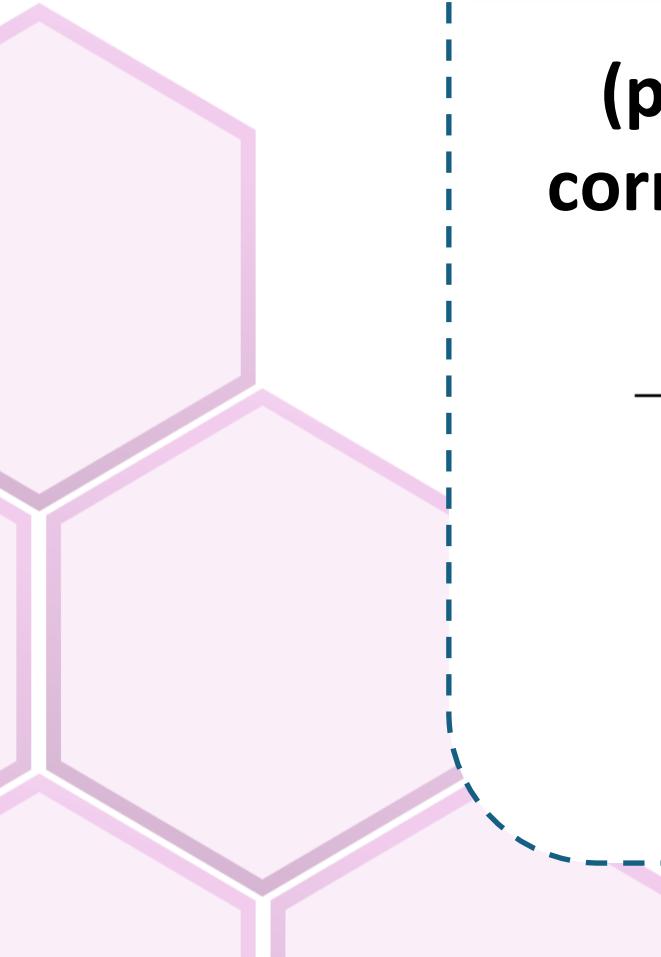
By solving the Schroedinger Equation

$$\hat{H}(\vec{r}, \vec{R}) \psi(\vec{r}, \vec{R}) = E \psi(\vec{r}, \vec{R})$$

$$\hat{H} = \hat{T}_e + \hat{T}_N + \hat{V}_{Ne} + \hat{V}_{ee} + \hat{V}_{NN}$$

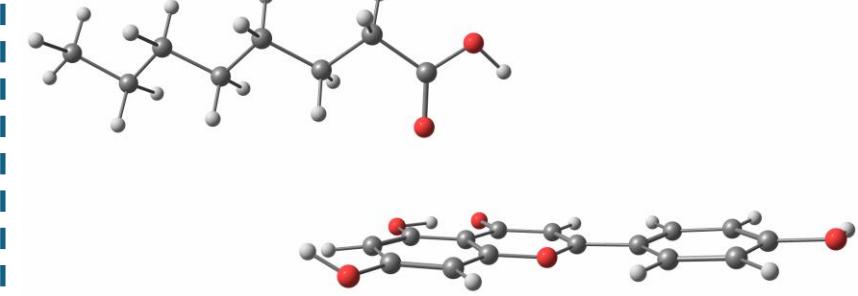
Many bodies → approximations and theories

# *Ab Initio* simulations - Density Functional Theory (DFT)

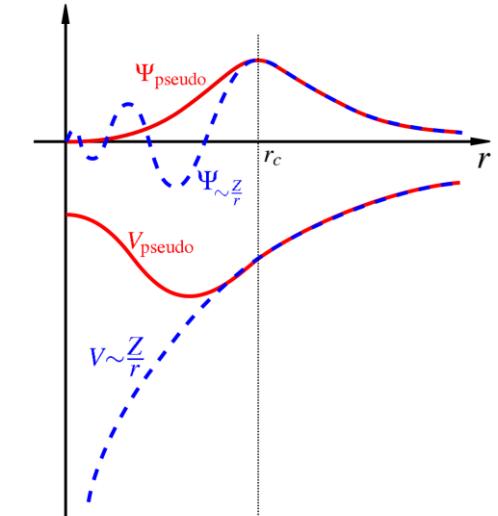


## Input

### 3D Files



### (pseudo/exchange correlation)potentials



## Simulation Codes

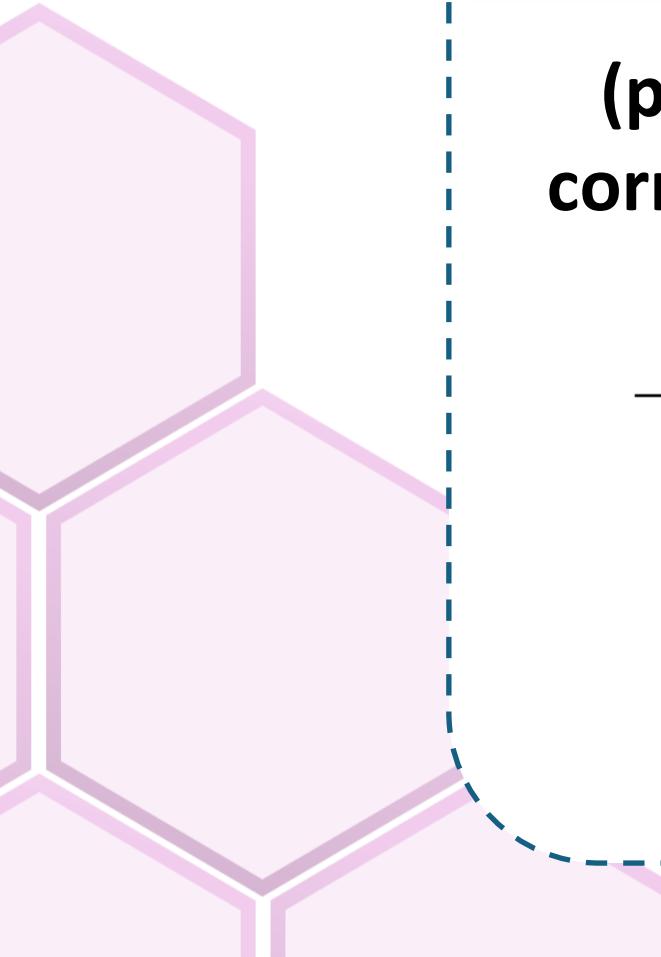


## Output

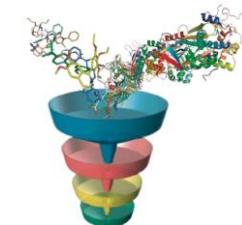
- Optimized atomic position
- Fundamental total energies
- Binding energies
- Charge transfers
- Electronic gap/HOMO-LUMO
- Band structures
- Transport properties
- Magnetic properties
- Vibrational properties



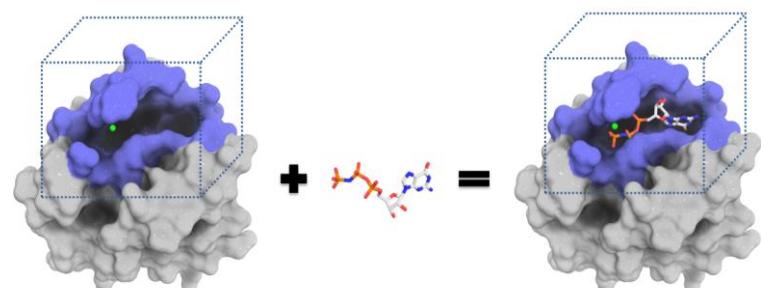
# *Ab Initio* simulations - Density Functional Theory (DFT)



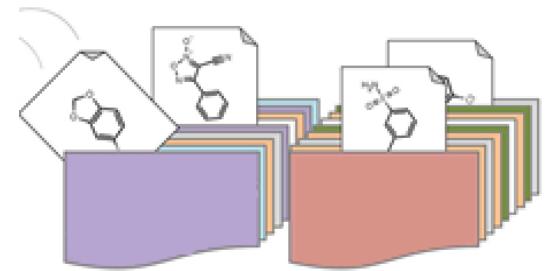
# Molecular Docking-Approach



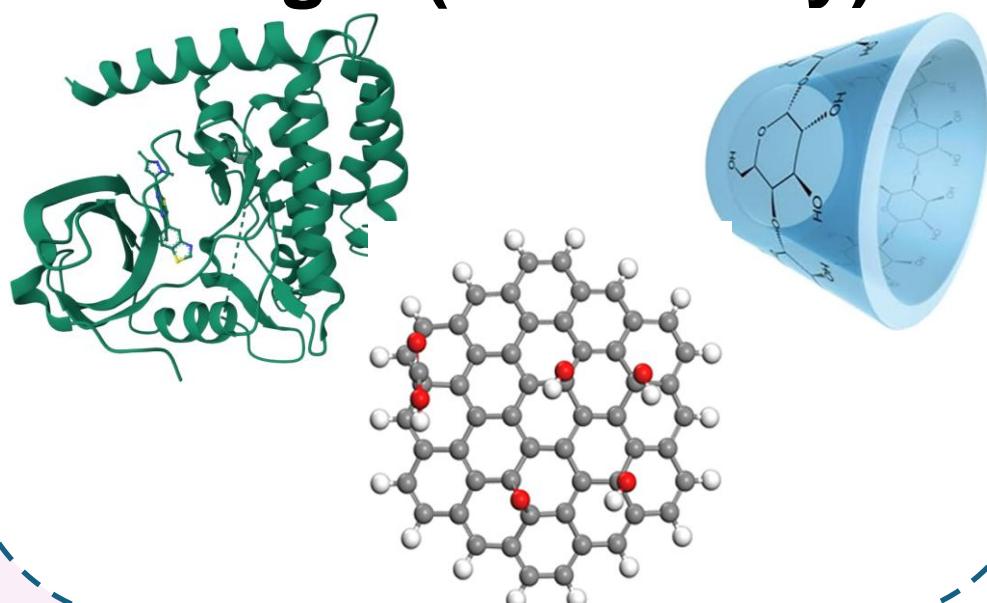
## Input



### Compounds – Ligands Virtual Screening



### Target (locker-key)



## Simulation Codes

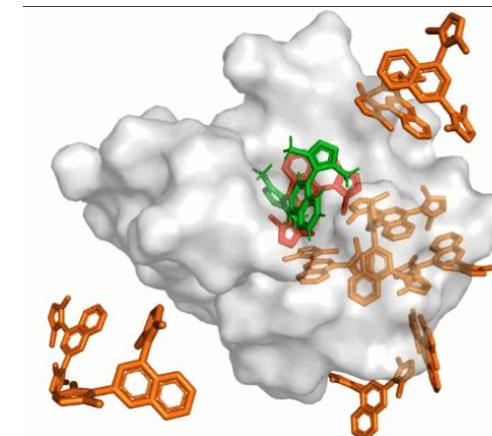
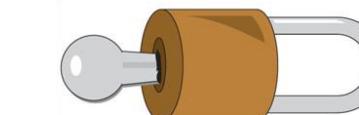


GOLD



AUTODOCK VINA

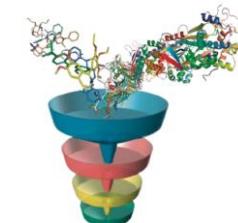
## Output



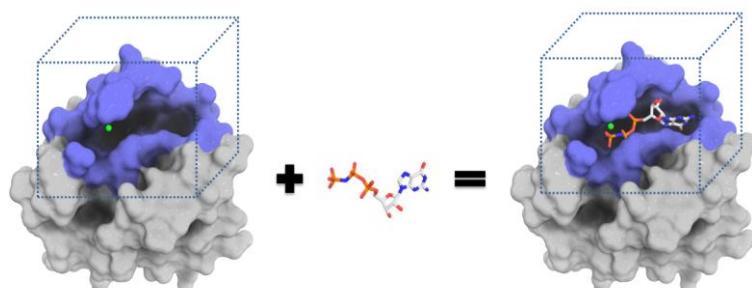
- Binding Energy
- Binding Poses
- Interaction Analysis (Molecular Contacts)
- Scoring and Ranking of Ligands
- Comparison with Known Drugs
- Prediction of Biological Activity
- Potential Drug Candidates for Further Study



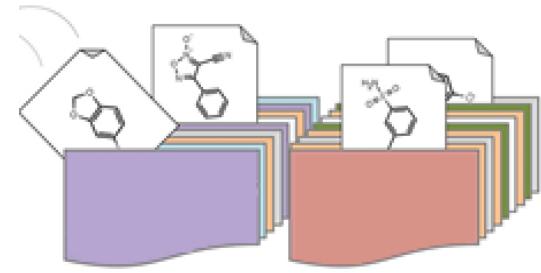
# Molecular Docking-Approach



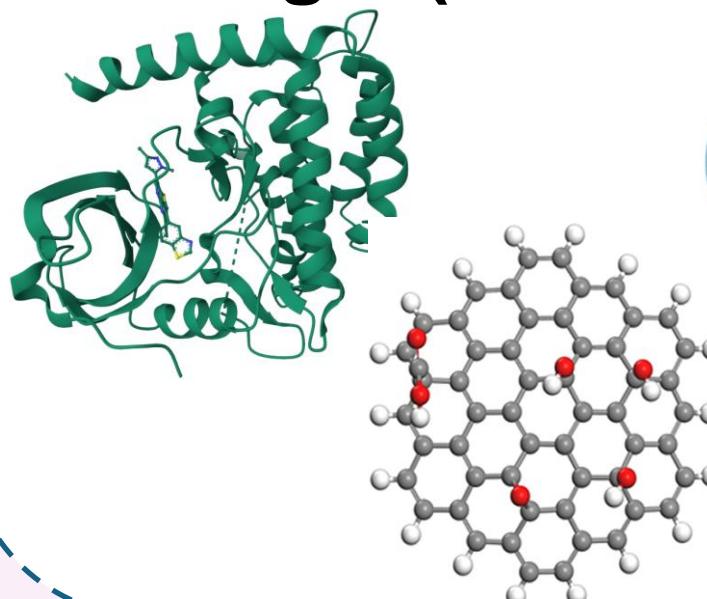
## Input



## Compounds – Ligands Virtual Screening



## Target (locker-key)



## Simulation Codes

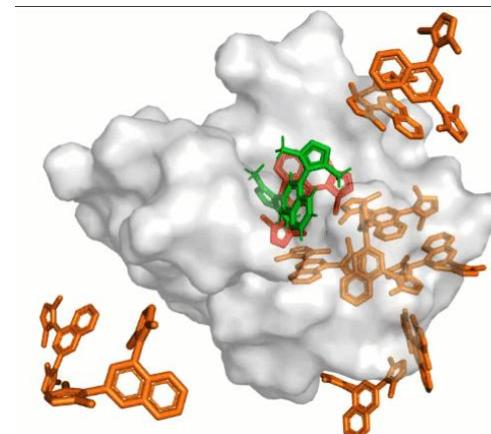


**IMPORTANT!!!**

- BIO INTERACTION INFORMATIONS
- HIGH NUMBER OF ATOMS
- SMALL COMPUTATIONAL COST
- DIFFICULT TO OBTAIN THE POTENTIALS
- LIMITED PHYSICAL AND CHEMICAL ANALYSES

**AUTODOCK VINA**

## Output



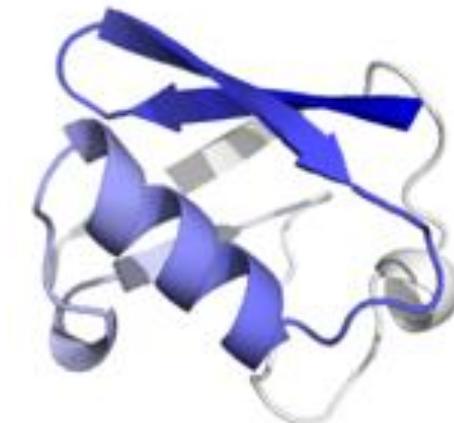
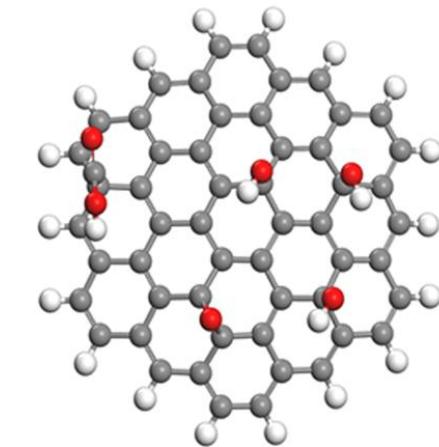
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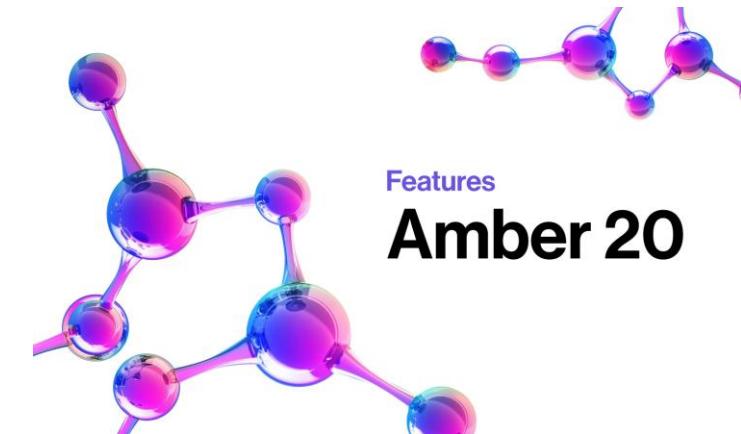
# Molecular Dynamics-Approach

## Input

- Temperature
- Pressure,
- Volume
- pH
- Type of solvent

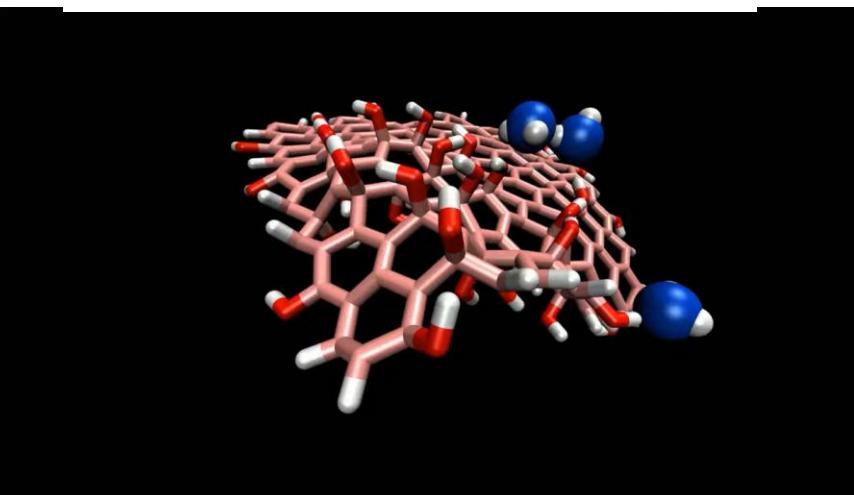


## Simulation Codes



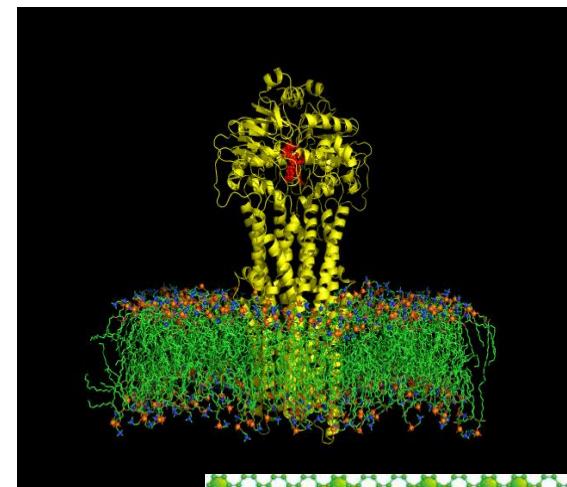
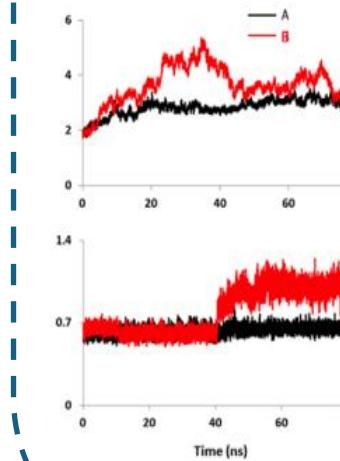
Features  
**Amber 20**

**GROMACS**  
fast, flexible & free



## Output

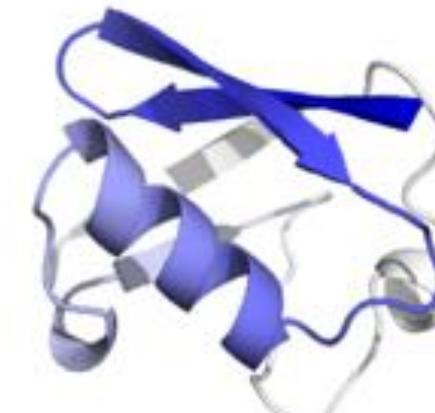
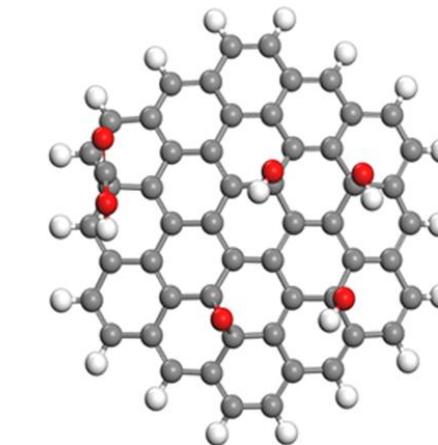
- Temporal trajectories
- Diffusion
- Mobility
- Potential energy
- Transition conformations
- Stability
- Temperature and pressure
- Solvation-solvent interactions
- Activation energies
- Reaction mechanisms



# Molecular Dynamics-Approach

## Input

- Temperature
- Pressure,
- Volume
- pH
- Type of solvent



## Simulation Codes



**IMPORTANT!!!**

- THERMODYNAMIC INFORMATIONS
- HIGH NUMBER OF ATOMS
- SMALL COMPUTATIONAL COST
- DIFFICULT TO HAVE THE POTENTIALS
- LIMITED PHYSICAL AND CHEMICAL ANALYSES



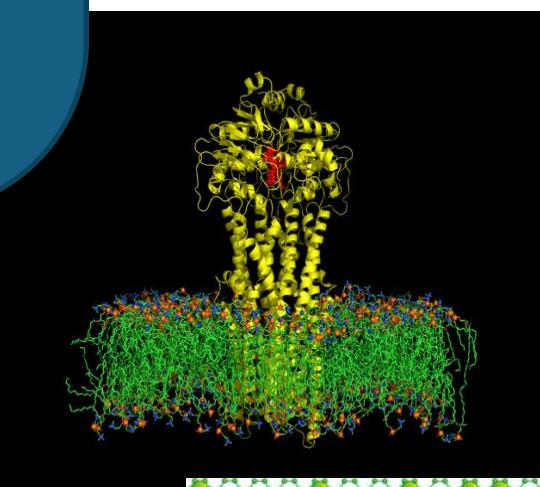
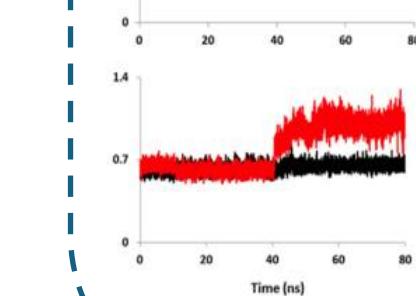
## Output

- Temporal trajectories
- Diffusion

Energy  
conformations

Time and pressure  
solvent

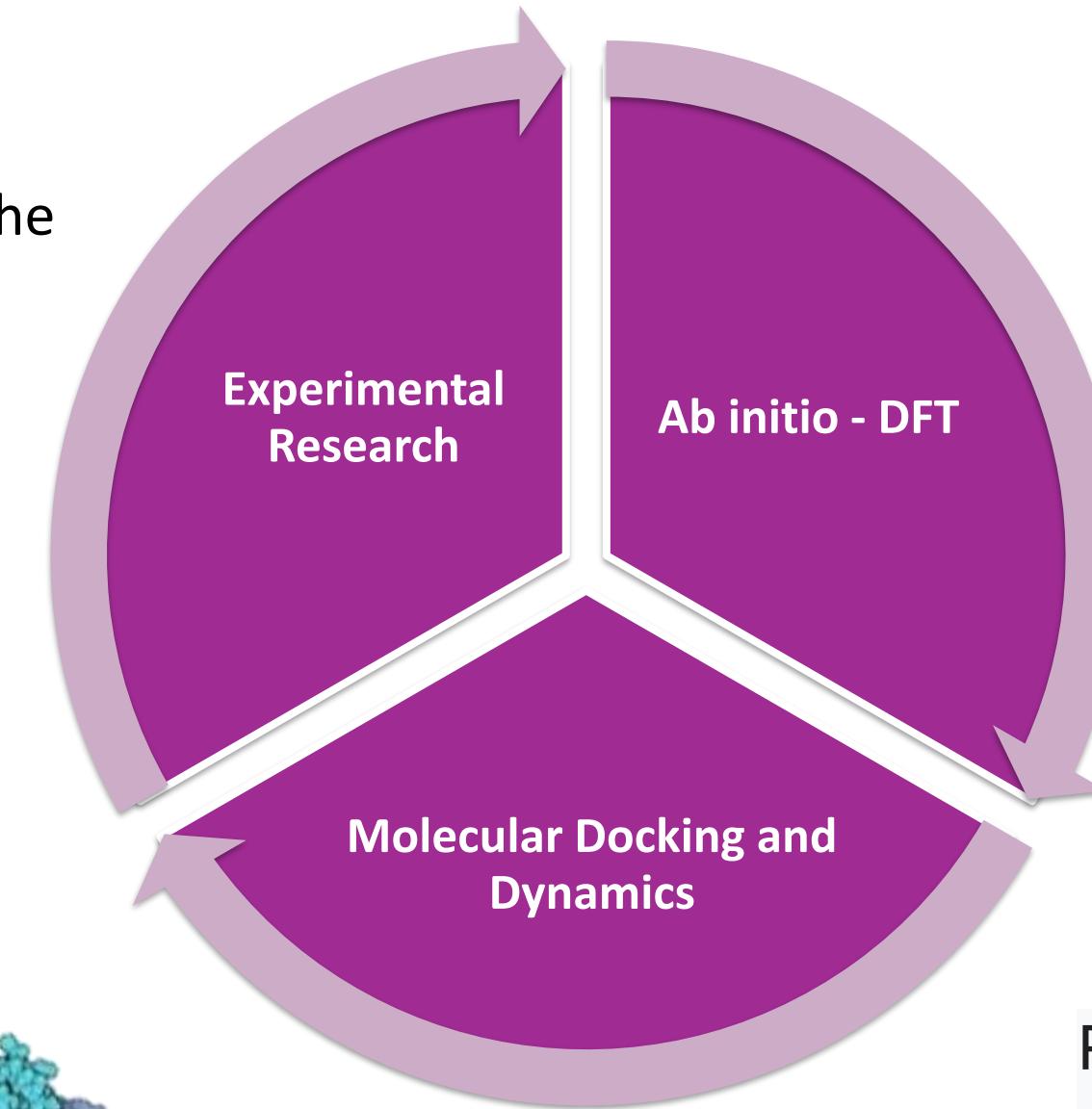
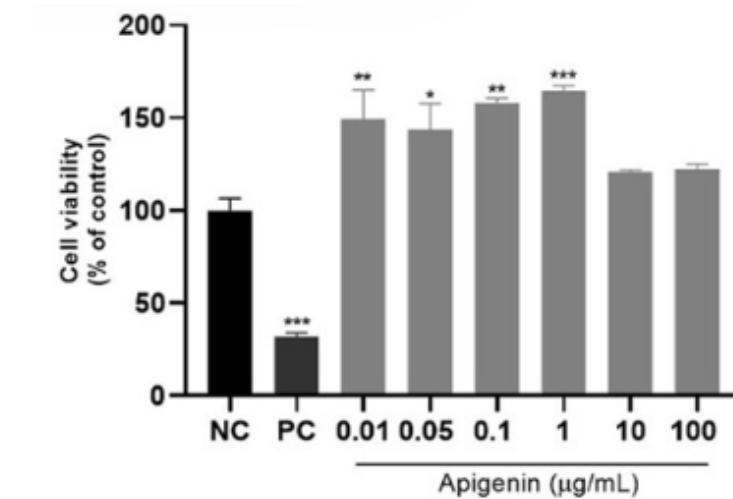
energies  
mechanisms



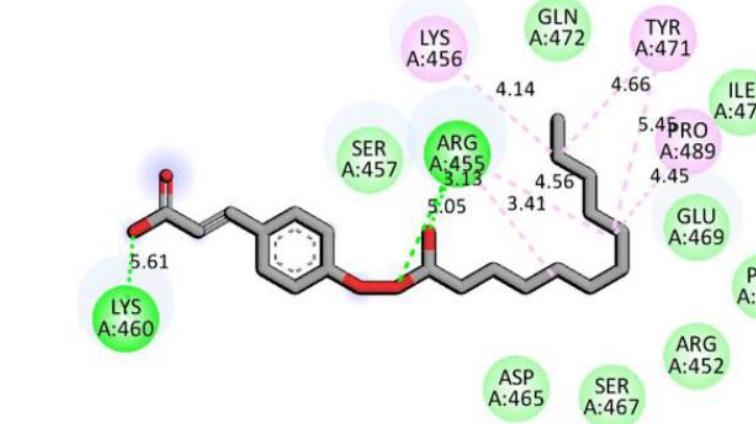
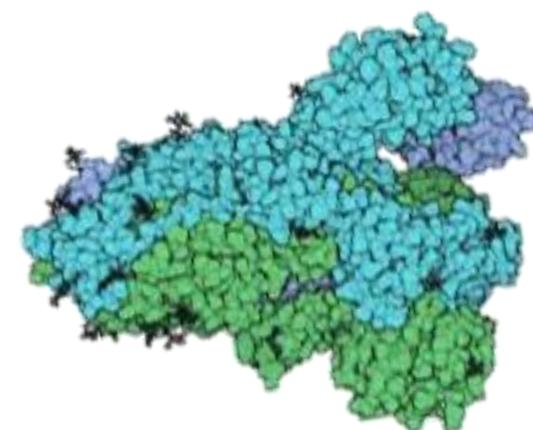
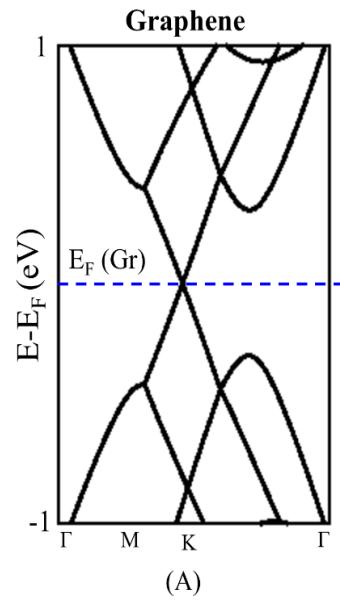
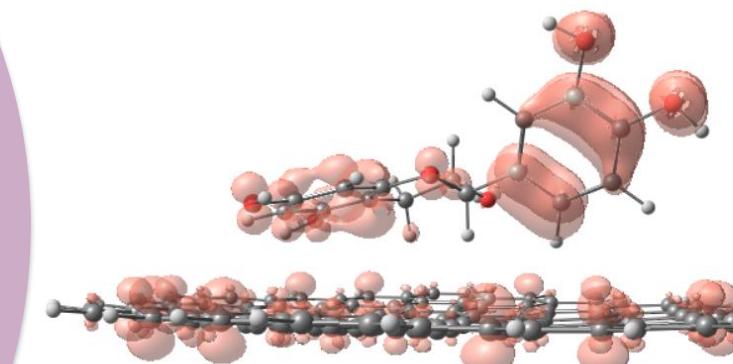
# SIMULATION/MODELING X EXPERIMENTAL CORRELATION

Experimental results of the best configurations

Simulation approach to understand the experiments

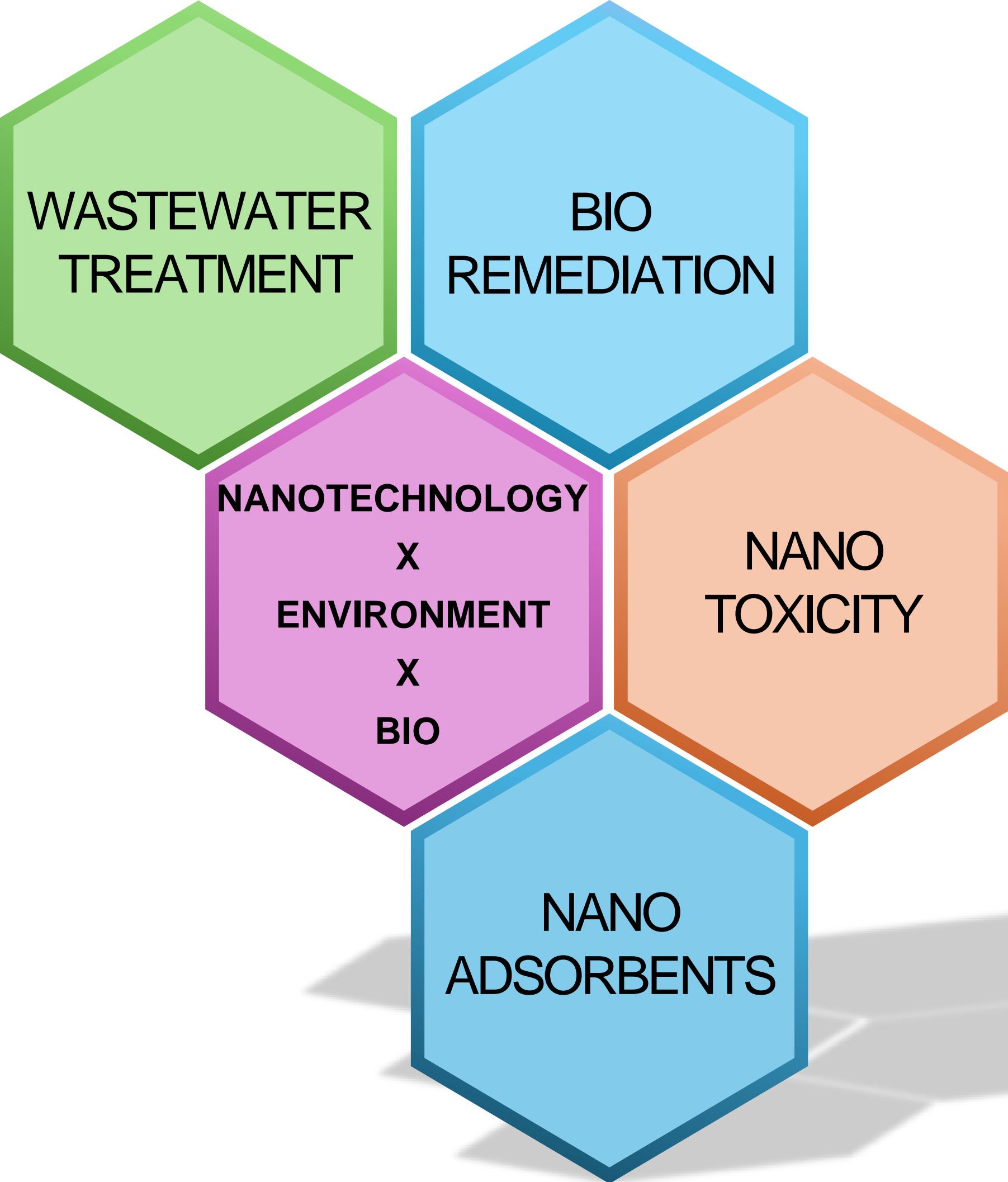


Interaction between molecules studied through **quantum mechanics**

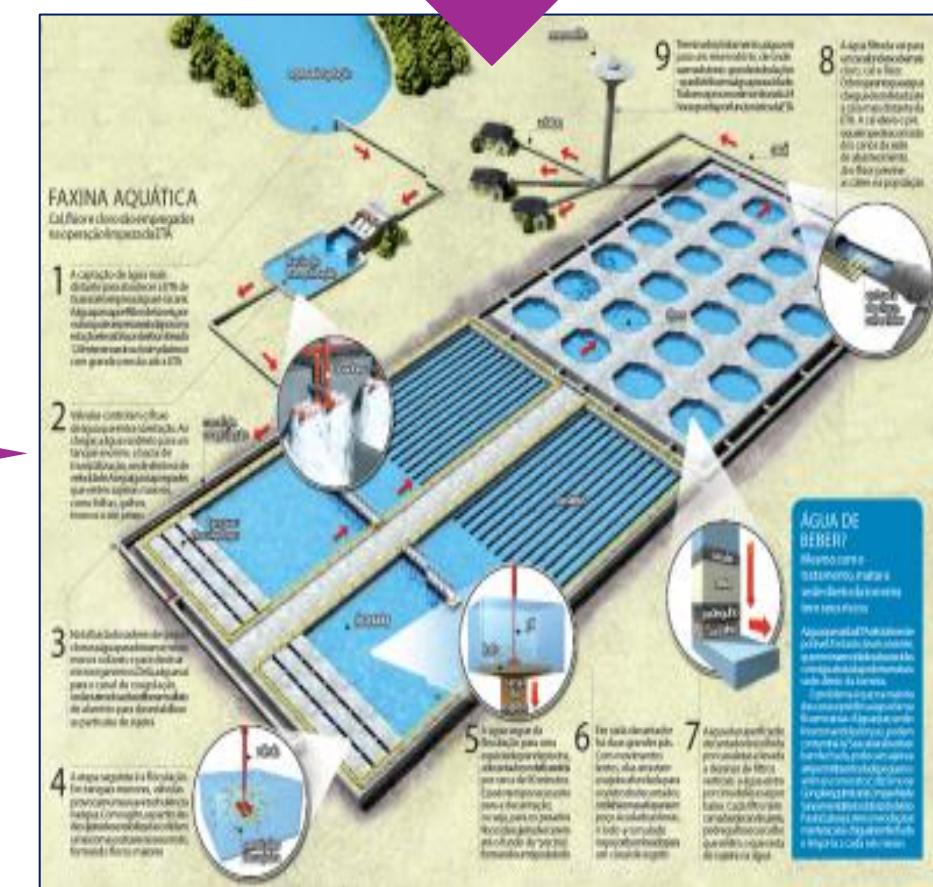
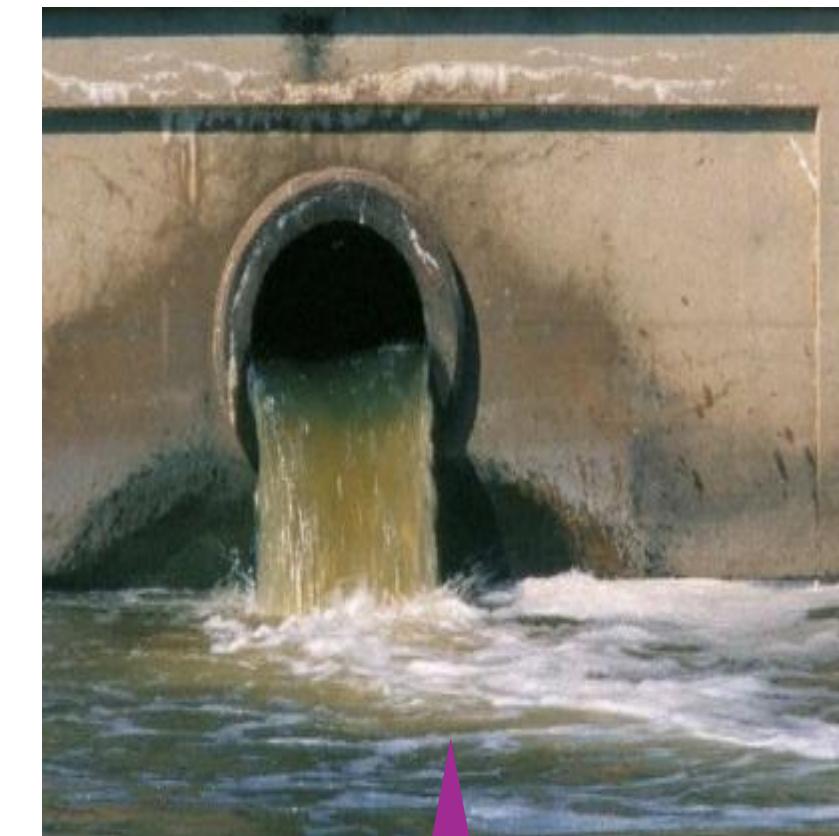
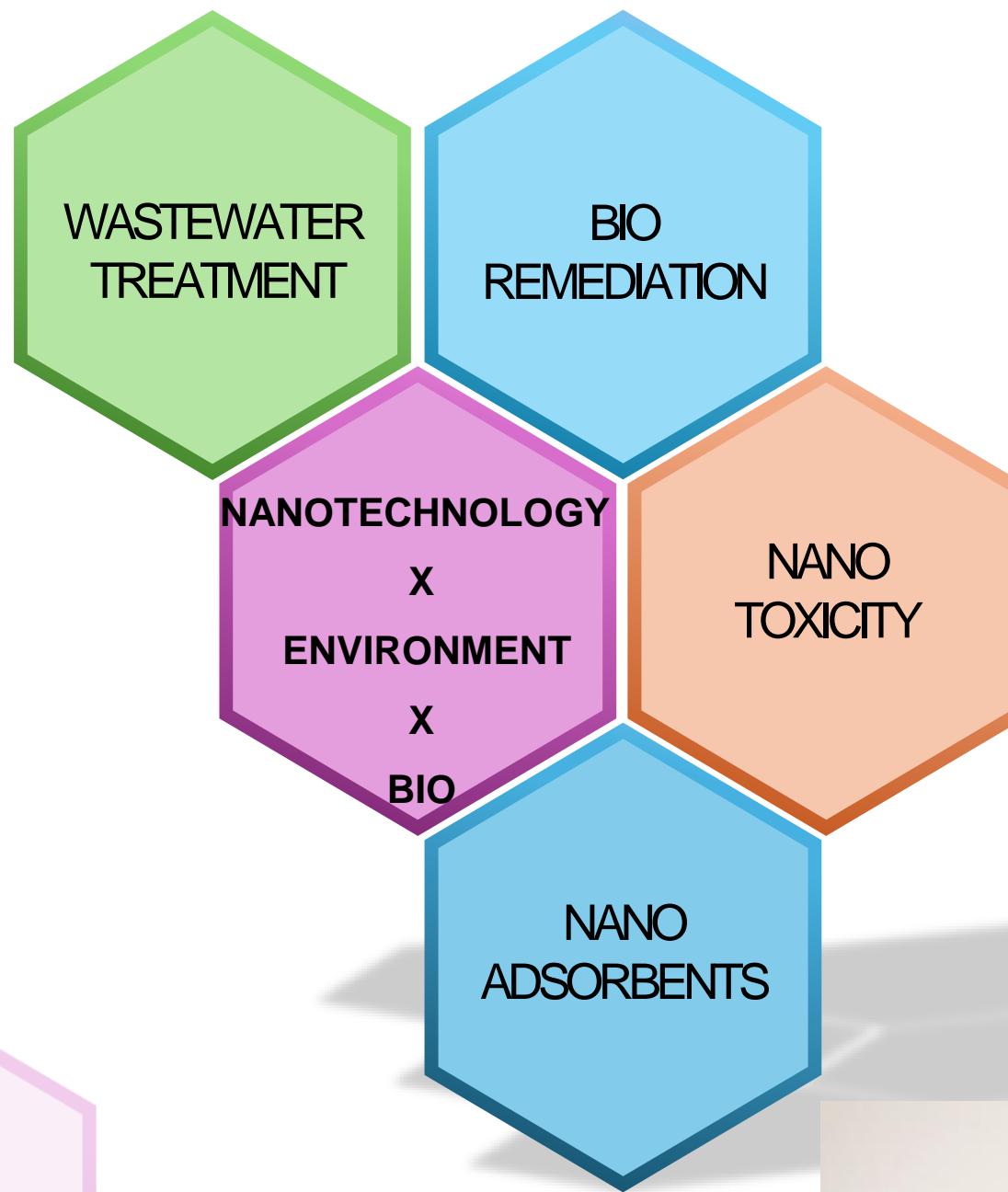


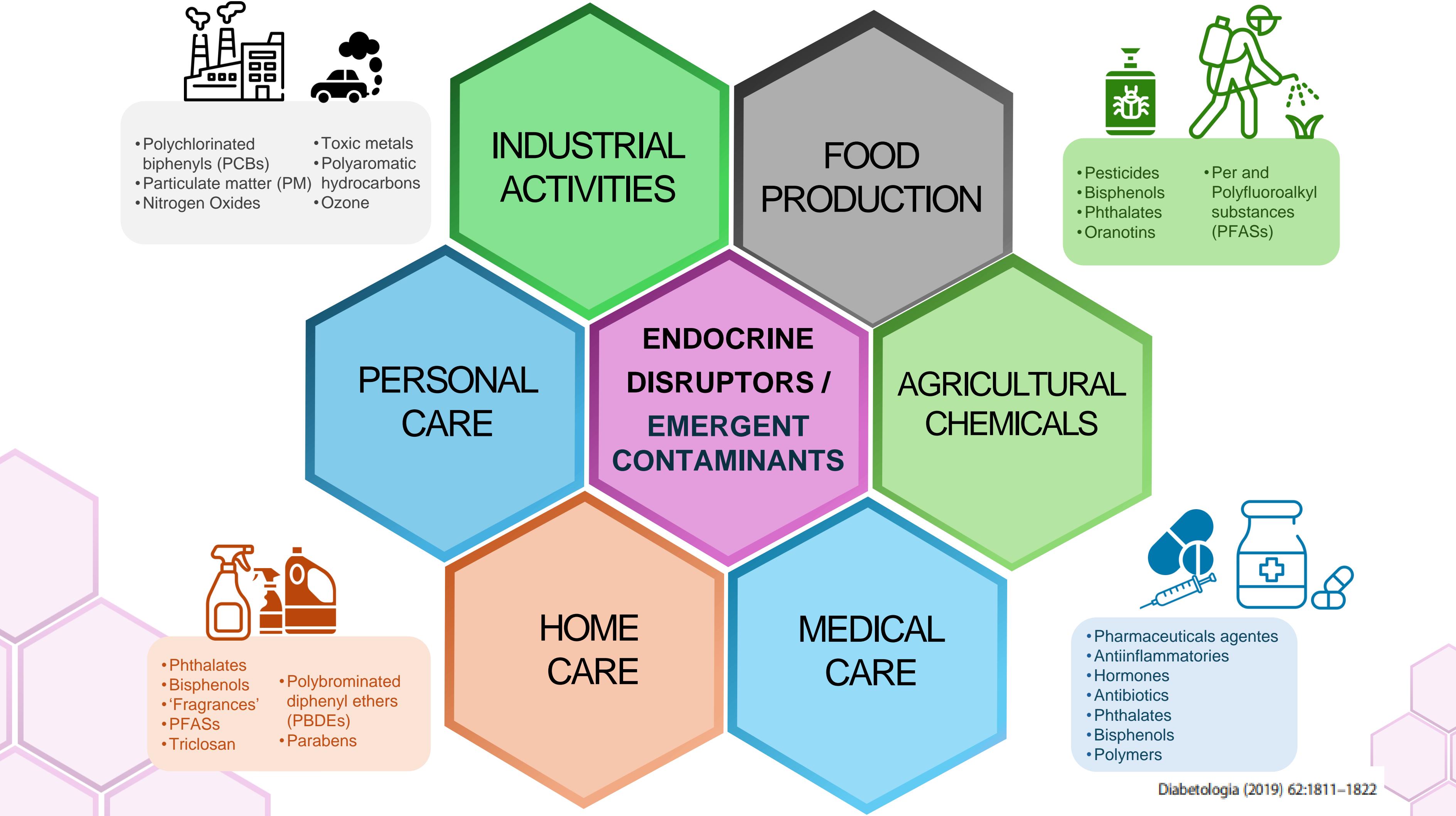
Predicts the interaction between two molecules, usually a protein and a ligand, to determine the best way in which they bind and the affinity between them.





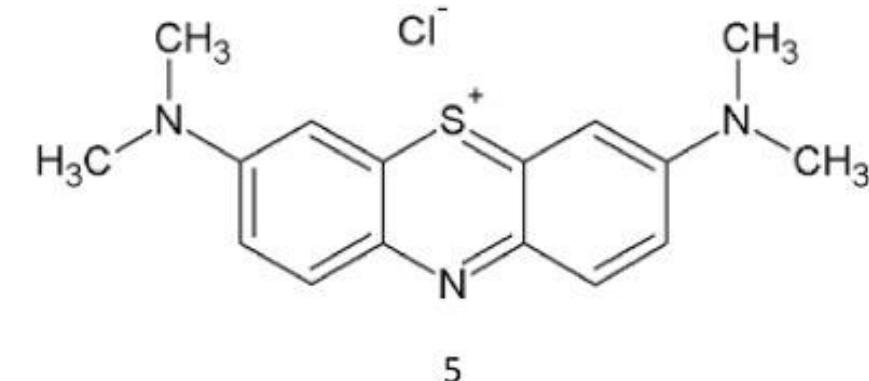
# ENDOCRINE DISRUPTORS OR EMERGENT CONTAMINANTS





## Combining multi-scale simulations and experiments to unveil the adsorption of methylene blue in graphene tridimensional-based materials

Mayara Bitencourt Leão, Laura Vendrame, Iuri Medeiros Jauris, Ivana Zanella, Solange Binotto Fagan, José Rafael Bordin and Carolina Ferreira de Matos



5



### Methylene Blue (MB) is used as a synthetic dye.

#### Major Uses:

- Paper and textile industries (wool, silk, cotton).
- Use in food, cosmetics, and pharmaceutical products.

#### Medicinal Effects:

- Safe usage when clinically prescribed.
- Risks when consumed through contaminated water.

#### Environmental and Human Health Impacts

- Discharge of wastewater containing MB from industries.
- Effects on humans: Cyanosis, Tissue necrosis  
Formation of Heinz bodies, Vomiting, jaundice, shock, and tachycardia
- Effects on plants: Growth inhibition, Reduced pigmentation, Decreased protein content in microalgae

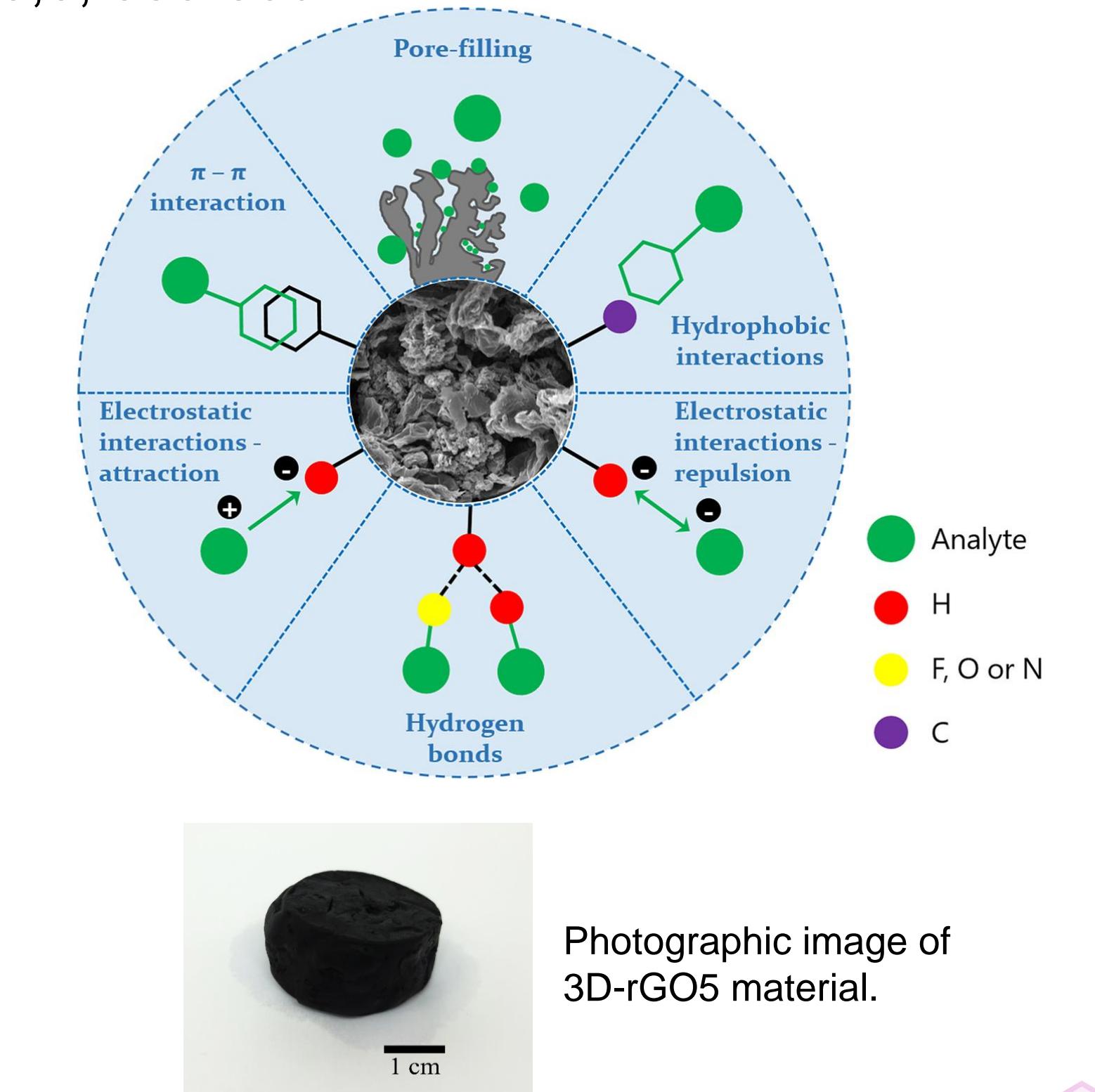
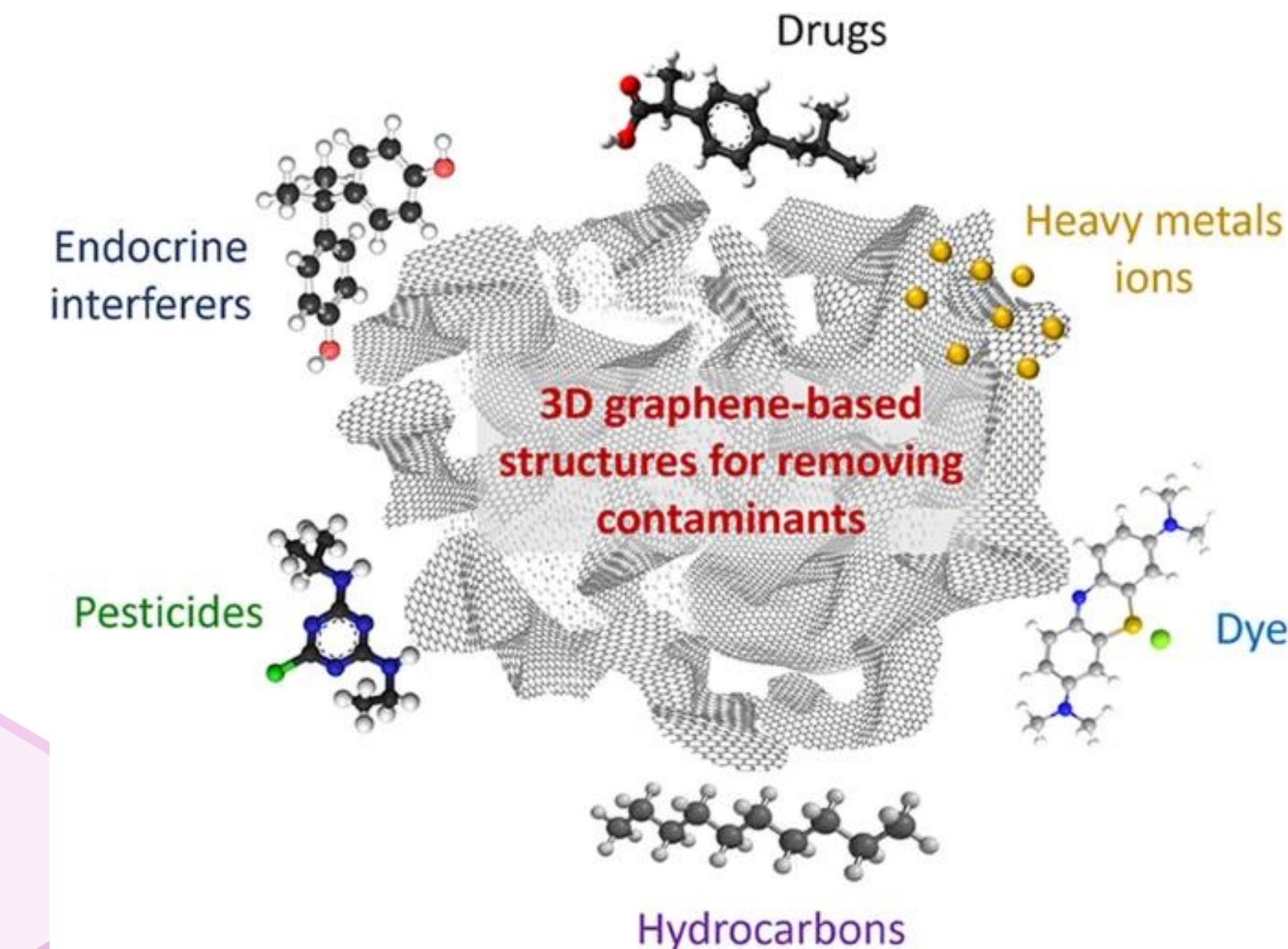
#### The Need for Efficient Removal:

- Importance of proper treatment before industrial discharge.
- Potential methods for removal and treatment.

Combining multi-scale simulations and experiments  
to unveil the adsorption of methylene blue in  
graphene tridimensional-based materials



Mayara Bitencourt Leão, Laura Vendrame, Iuri Medeiros Jauris, Ivana Zanella, Solange Binotto Fagan, José Rafael Bordin and  
Carolina Ferreira de Matos



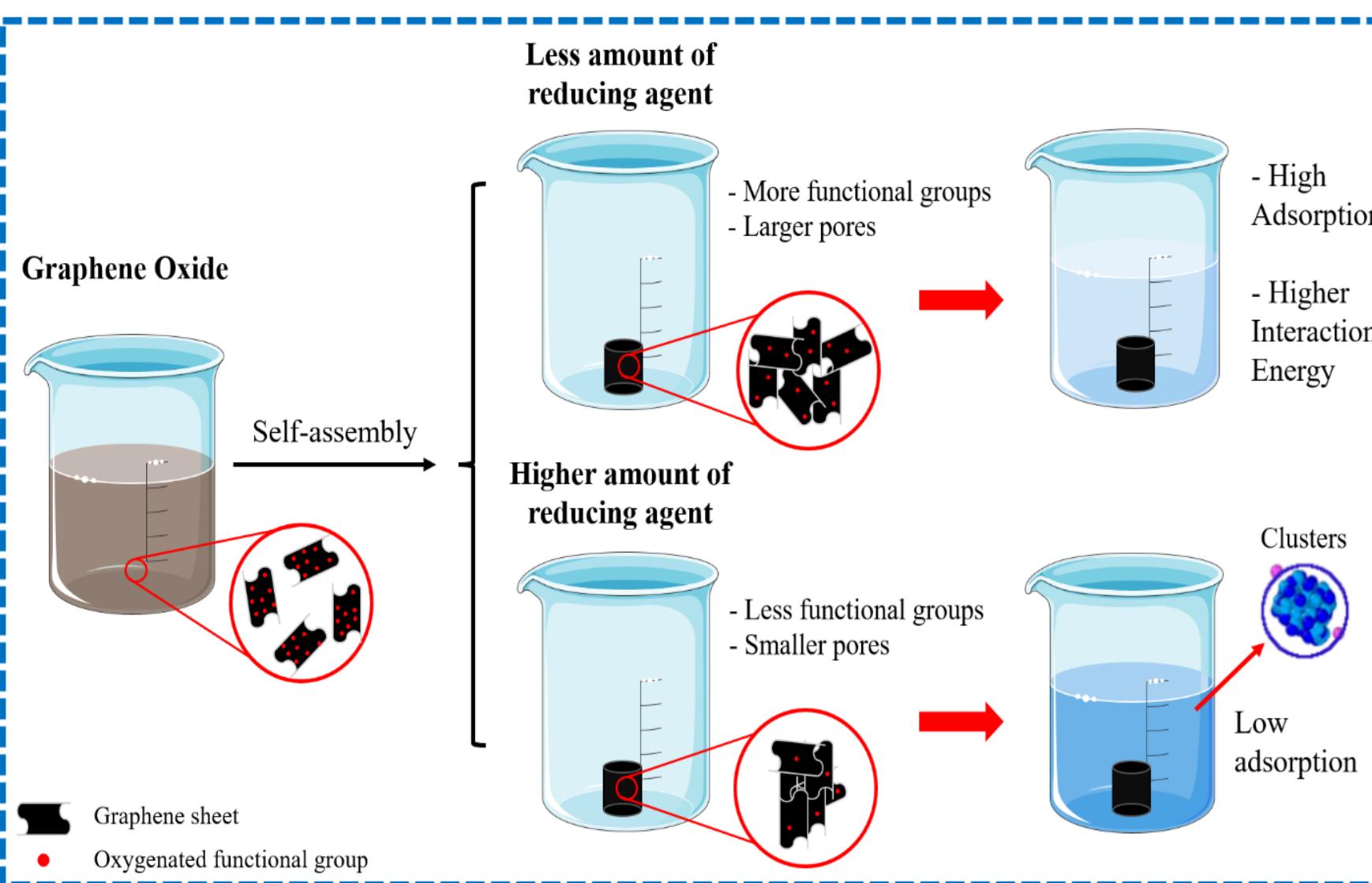
Specific Surface Area Versus Adsorptive Capacity: an Application View of 3D Graphene-Based Materials for the Removal of Emerging Water Pollutants



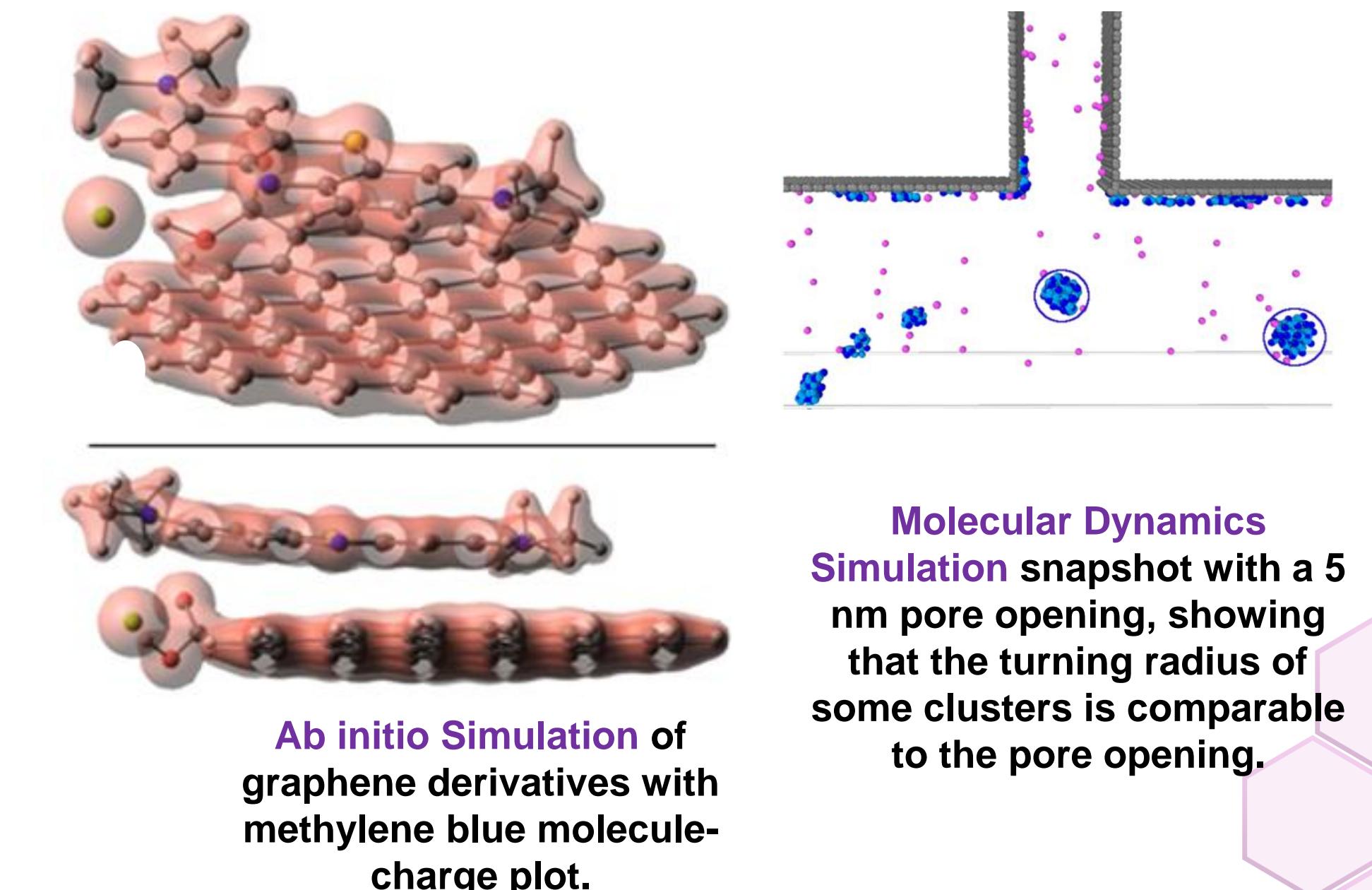
Combining multi-scale simulations and experiments  
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[Mayara Bitencourt Leão](#), [Laura Vendrame](#), [Juri Medeiros Jauris](#), [Ivana Zanella](#), [Solange Binotto Fagan](#), [José Rafael Bordin](#) and  
[Carolina Ferreira de Matos](#)

## Adsorption of methylene blue dye onto 3D graphene containing different amounts of reducing agent and, consequently, different pore sizes and degrees of oxidation.



- **Physical adsorption**, being dependent on the presence of functional groups on the graphene surface (**reusable**).
- The intensity of physical adsorption depends on the presence of functional groups in the graphene surface, **increasing as the number of epoxy and hydroxy functional groups increase** and decreasing when carboxyl functional groups increase.
- This indicates that the most significant difference between the materials is related to their morphology but is also influenced by the presence of oxygenated groups.

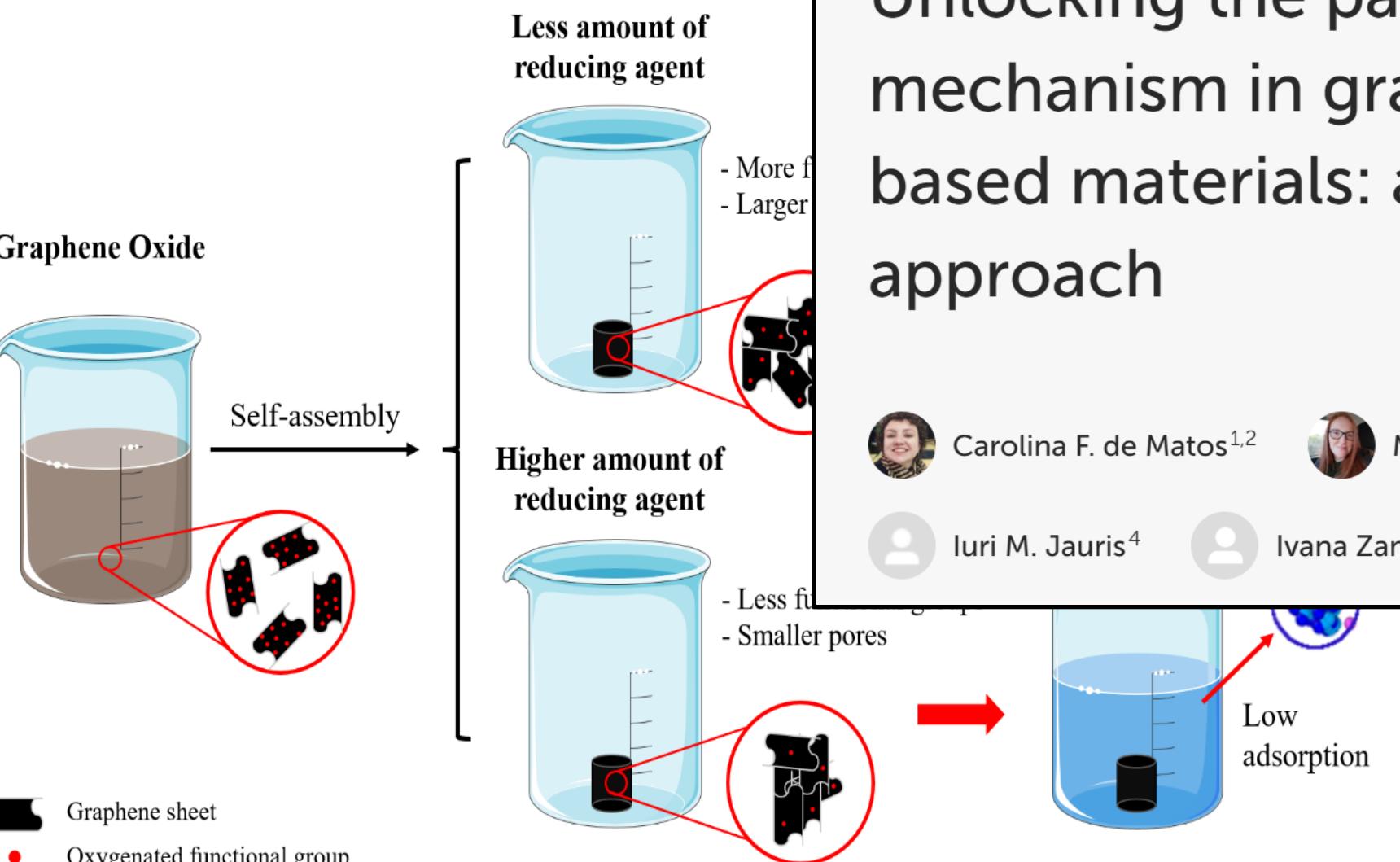




Combining multi-scale simulations and experiments  
to unveil the adsorption of methylene blue in  
graphene tridimensional-based materials

Mayara Bitencourt Leão, Laura Vendrame, Juri Medeiros Jauris, Ivana Zanella, Solange Binotto Fagan, José Rafael Bordin and  
Carolina Ferreira de Matos

## Adsorption of methylene blue on graphene containing different amounts of reducing agent and, consequently, different degrees of oxidation



### ORIGINAL RESEARCH article

Front. Carbon, 04 February 2024  
Sec. Graphite-ene  
Volume 3 - 2024 |  
<https://doi.org/10.3389/frcrb.2024.1305183>

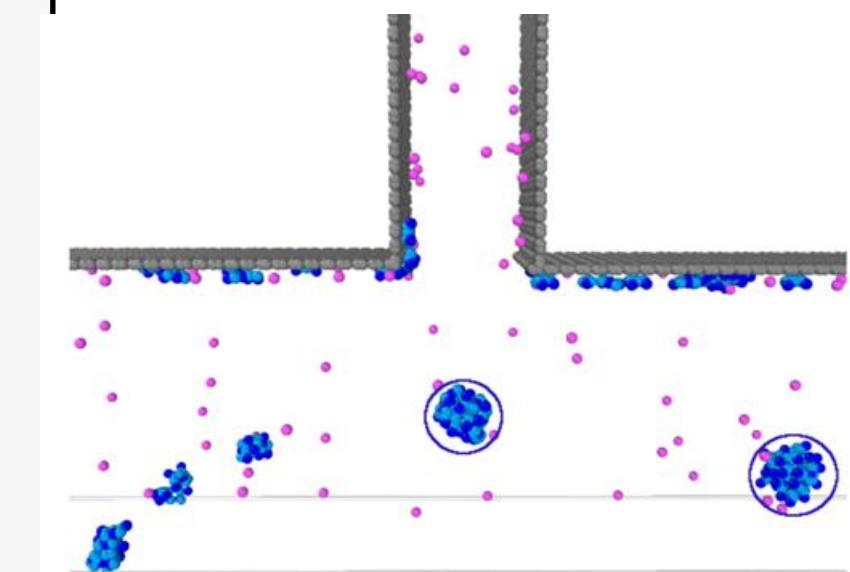
- **Physical adsorption**, being dependent on the presence of functional groups on the graphene surface (**reusable**).
- The intensity of physical adsorption depends on the presence of functional groups in the graphene surface, **increasing as the number of epoxy and hydroxy functional groups increase** and **functional groups increase**.

can difference between the technology but is also influenced by groups.

## Unlocking the paracetamol adsorption mechanism in graphene tridimensional-based materials: an experimental-theoretical approach

Carolina F. de Matos<sup>1,2</sup> Mayara B. Leão<sup>1</sup> Laura F. O. Vendrame<sup>3</sup>

Iuri M. Jauris<sup>4</sup> Ivana Zanella<sup>3</sup> Solange B. Fagan<sup>3\*</sup>



**Molecular Dynamics Simulation** snapshot with a 5 nm pore opening, showing that the turning radius of some clusters is comparable to the pore opening.

**Ab initio Simulation** of graphene derivatives with methylene blue molecule-charge plot.

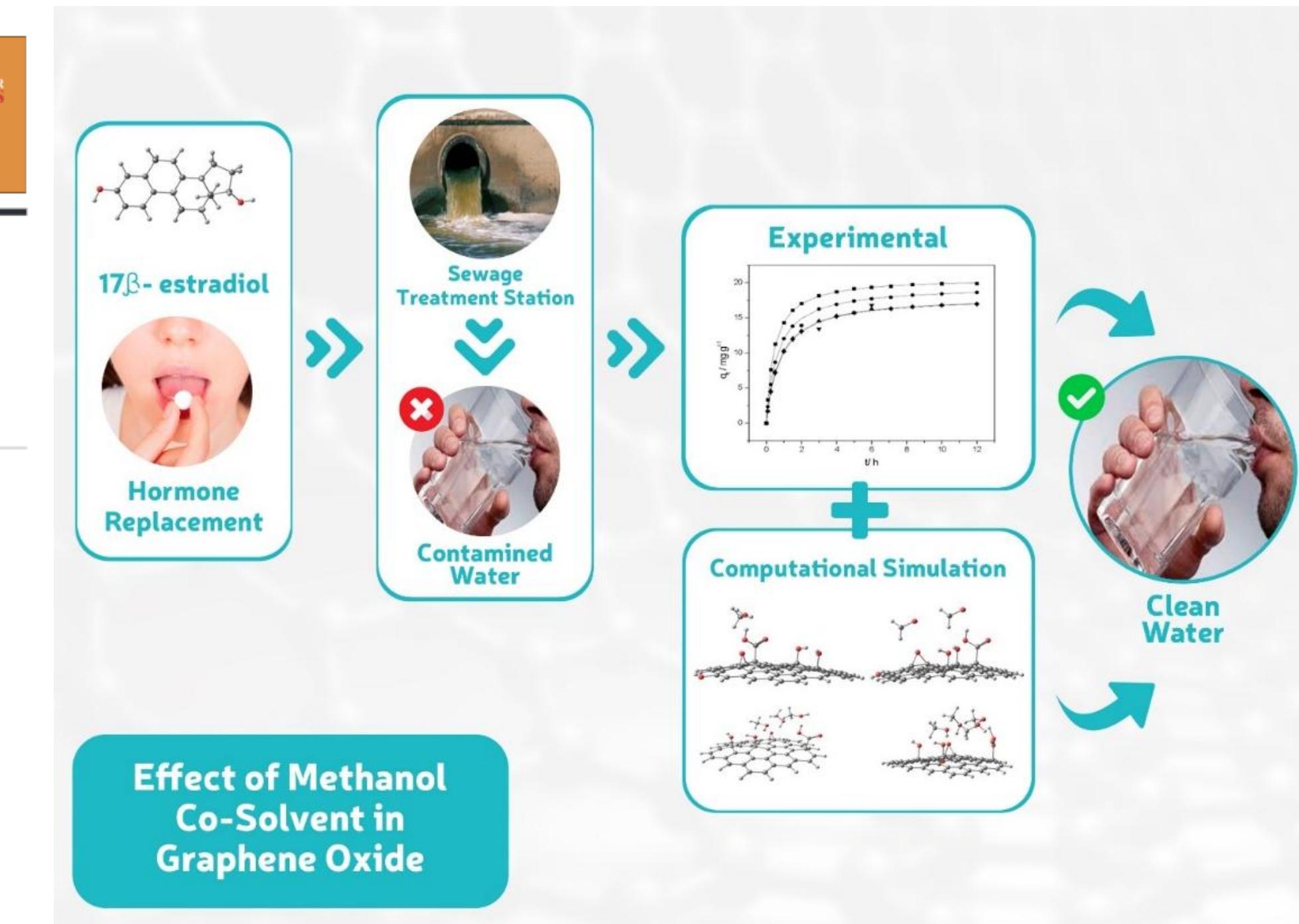
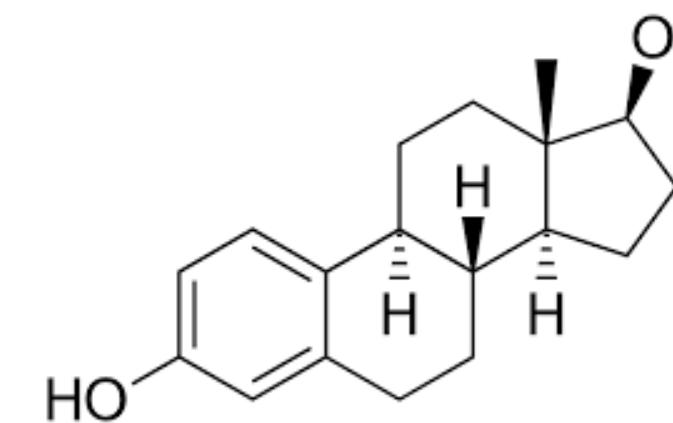




## Adsorption of $17\beta$ -estradiol in graphene oxide through the competing methanol co-solvent: Experimental and computational analysis

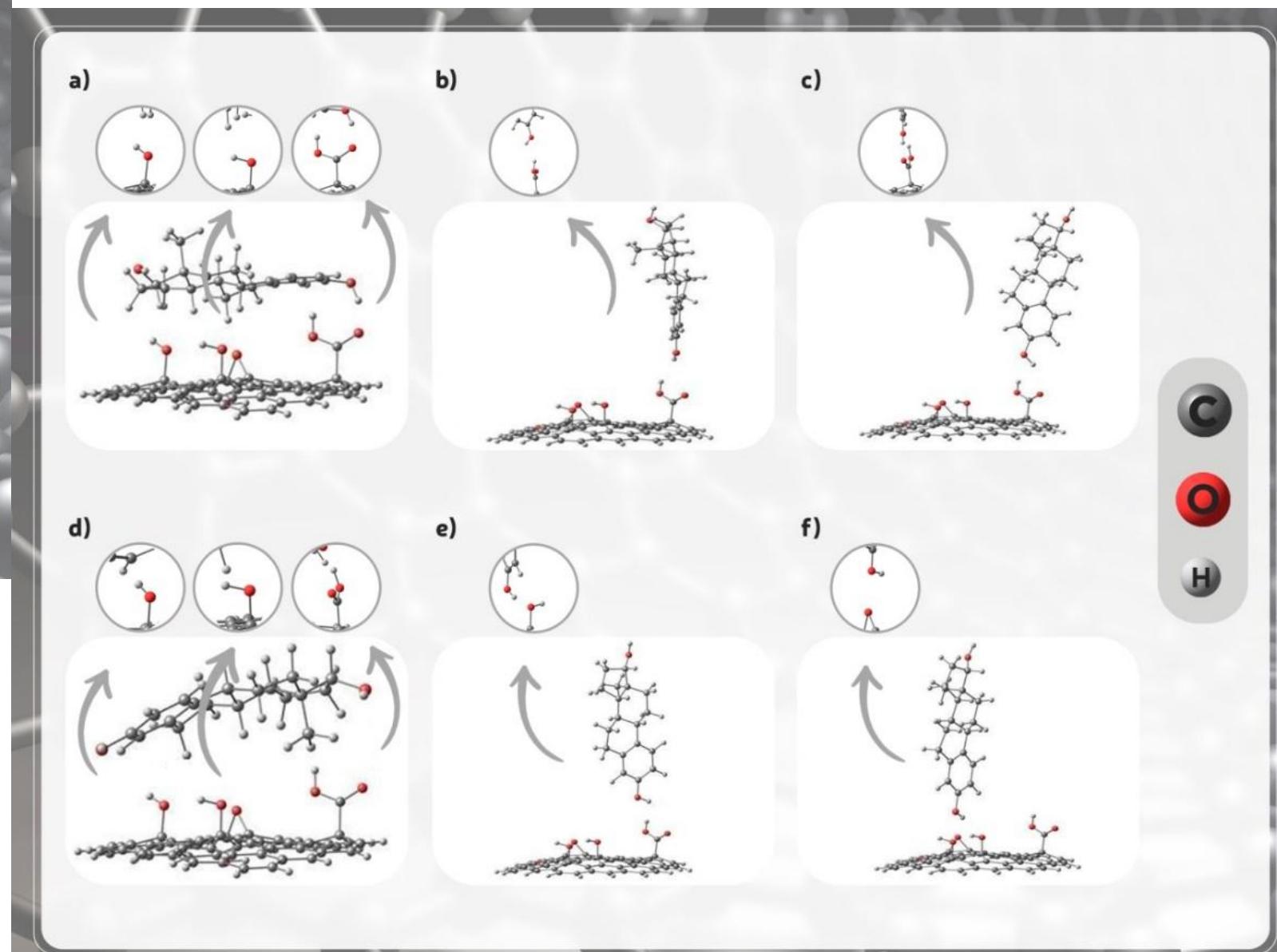
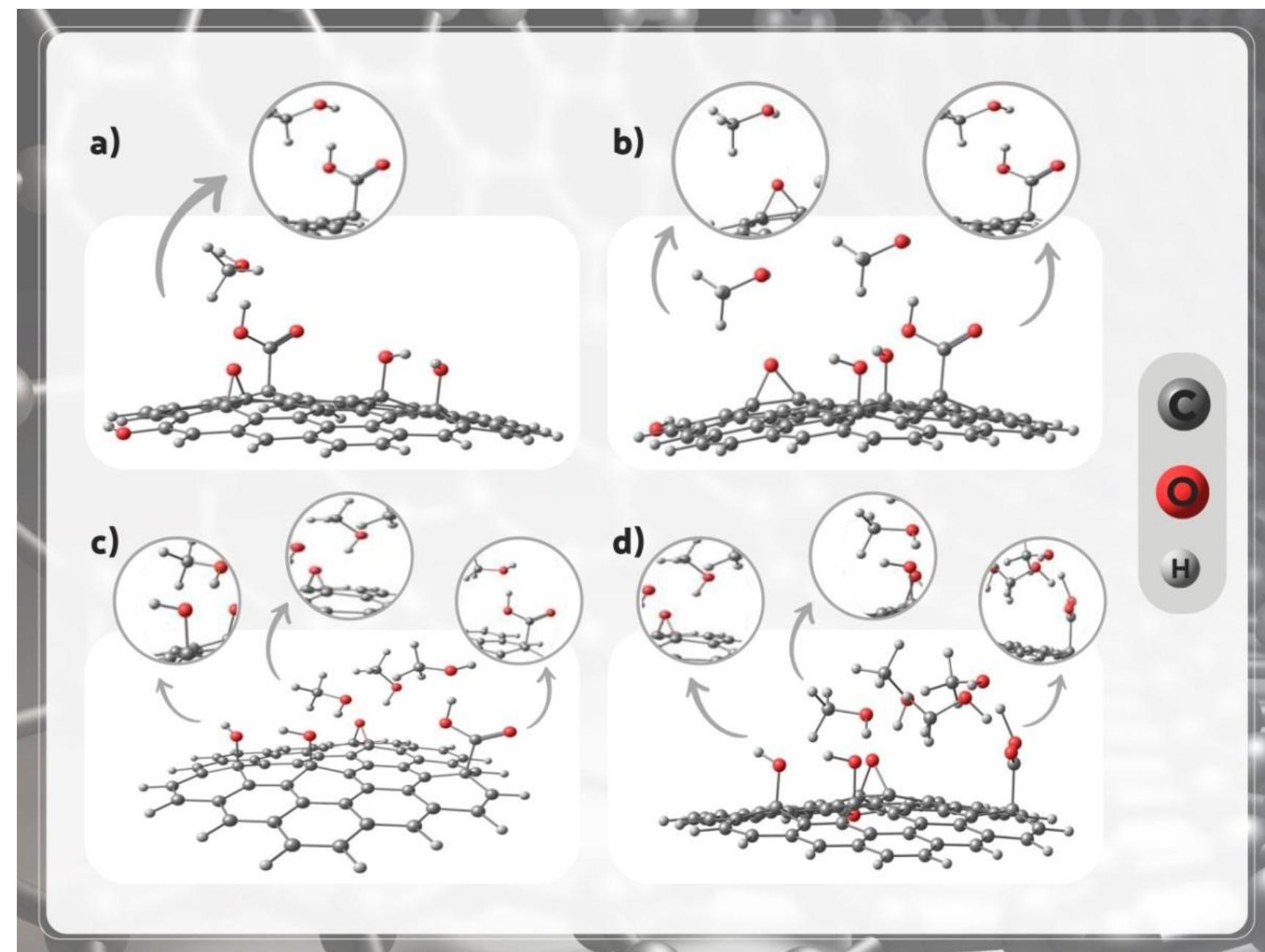
Patrícia Viera de Oliveira, Ivana Zanella \*, Luís Otávio S. Bulhões, Solange Binotto Fagan

Area of Technological Sciences, Universidade Franciscana, UFN, 970010-032 Santa Maria, RS, Brazil



- Methanol co-solvent competes with the **adsorption process** on graphene oxide.
- Highest  $17\beta$ -estradiol **removal** with the minimal methanol amount.
- The adsorption mechanism occurs by  **$\pi-\pi$  interactions** and physical adsorption.

# AB INITIO SIMULATIONS

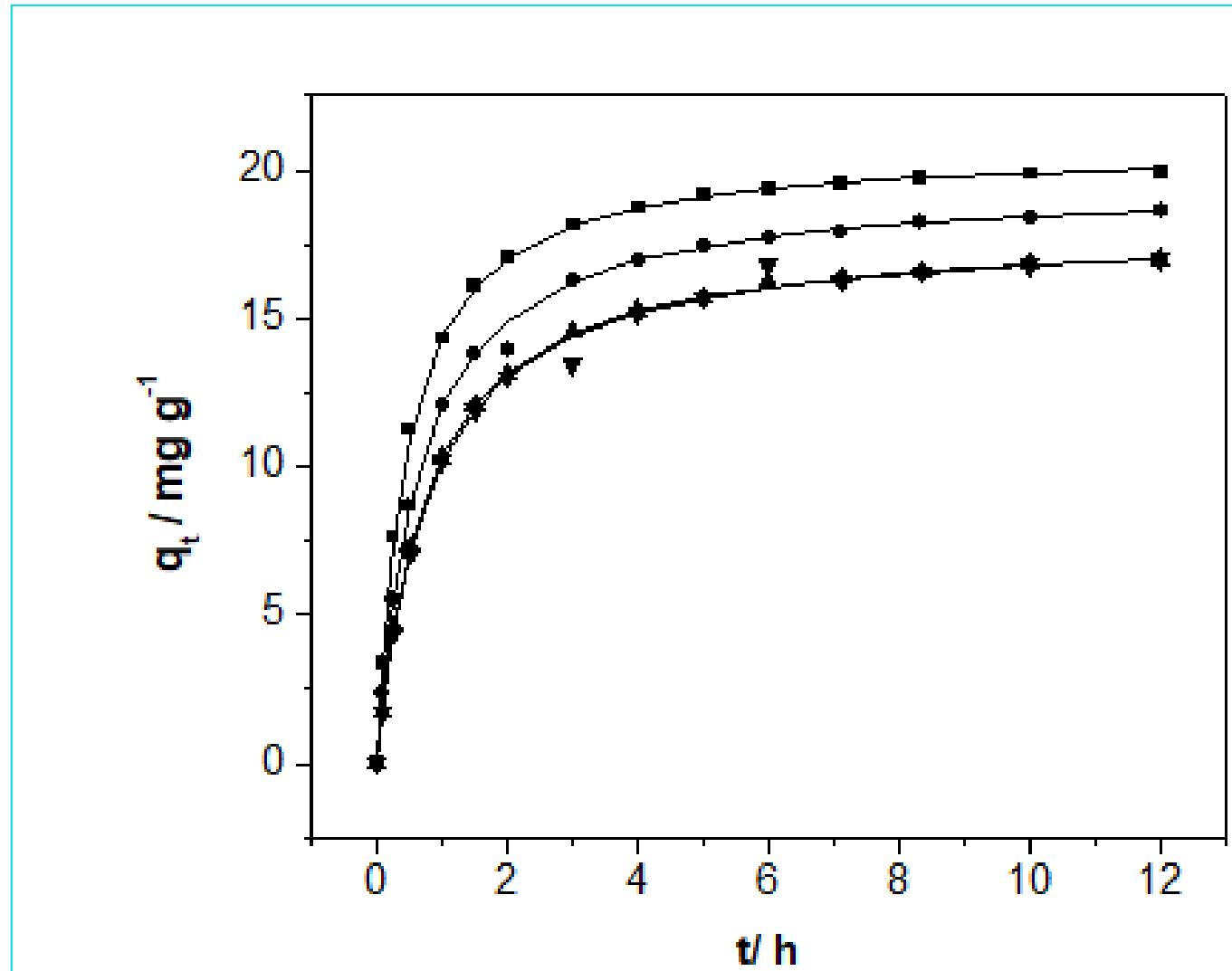


# SIMULATION RESULTS

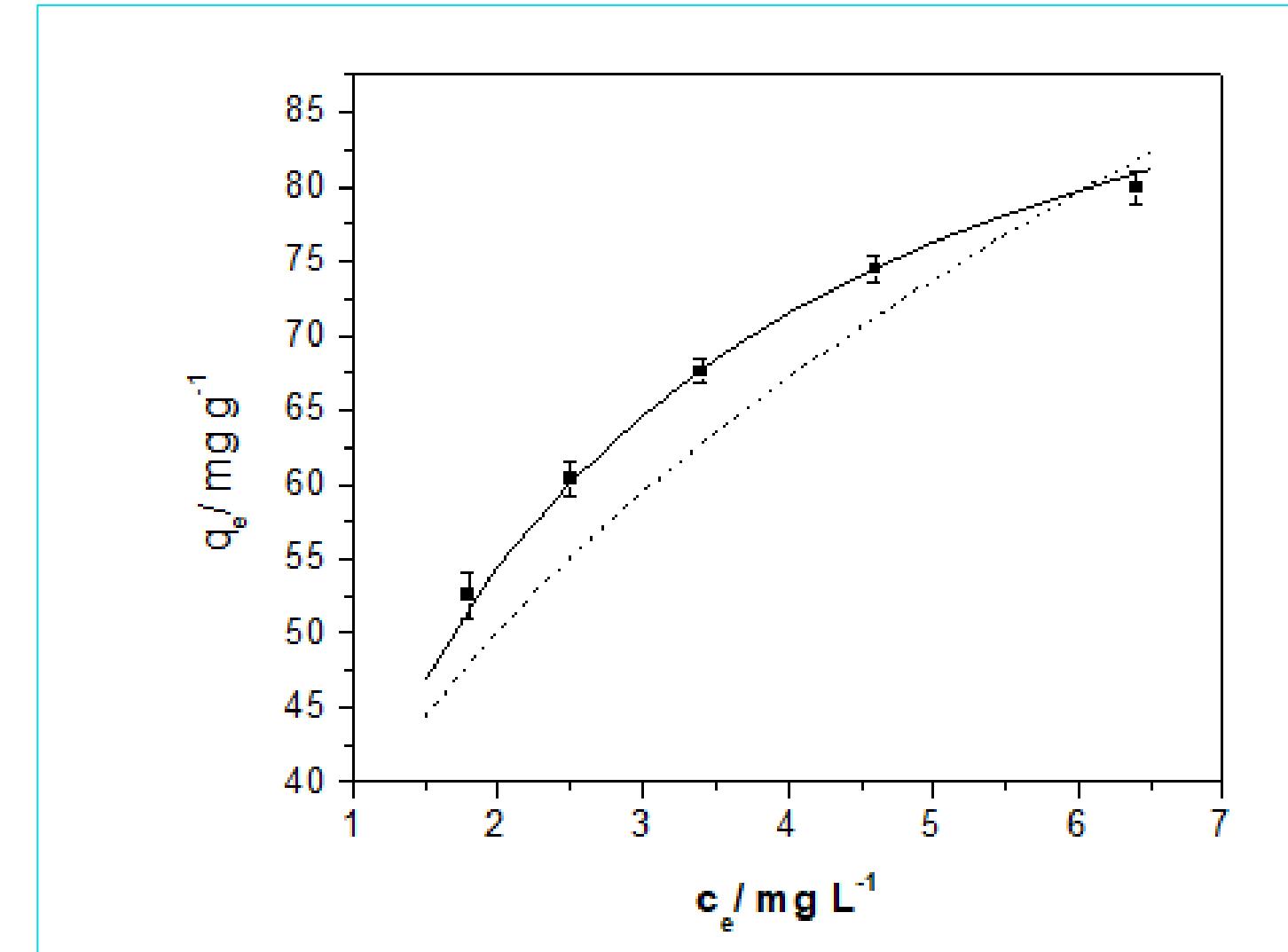
Configuration	Nº methanol molecules	D (Å)	E <sub>ads</sub> (eV)	ΔHL (eV)	ΔQ <sub>total</sub> (e-)	ΔQ per molecule of Methanol (e-)
Methanol	-	-	-	1.59	-	-
Graphene oxide	-	-	-	0.44	-	-
Graphene oxide +Methanol	1	2.00 C-H	0.45	0.56	-0.19	-0.19
Graphene oxide +Methanol	2	1.47 O-H	0.41	0.49	-0.09	-0.188/+0.096
Graphene oxide +Methanol	3	1.42 O-H	0.55	0.76	+0.01	+0.100/-0.170/+0.080
<b>Graphene oxide +Methanol</b>	<b>4</b>	<b>1.12 O-H</b>	<b>1.08</b>	<b>0.77</b>	<b>-0.05</b>	<b>+0.074/-0.056/-0.172/+0.104</b>

Configurations	D (Å)	E <sub>ads</sub> (eV)	ΔHL (eV)	ΔQ (e-)
GO	-	-	0.44	-
17 $\beta$ -estradiol	-	-	3.99	-
GO <sub>+</sub> 17 $\beta$ -estradiol (A)	1.64 O-H	1.28	0.25	0
GO+17 $\beta$ -estradiol (B)	2.60 O-H	0.06	0.26	-0.67
GO+17 $\beta$ -estradiol (C)	1.53 O-H	1.02	0.26	+0.03
<b>GO+17<math>\beta</math>-estradiol (D)</b>	<b>1.43 O-H</b>	<b>1.88</b>	<b>0.26</b>	<b>-0.09</b>
GO+17 $\beta$ -estradiol (E)	1.66 O-H	0.56	0.58	+0.15
GO+17 $\beta$ -estradiol (F)	1.91 O-H	0.22	0.61	+0.05

# ADSORPTION RESULTS (FROM EXPERIMENTS)



Kinetics of adsorption of 17 $\beta$ -estradiol in water-methanol solution (■) 98:2; (●) 90:10; ( $\blacktriangle$ ) 70:30 (▼) 50:50 % (m/m) at 288K, fitted with pseudo-second order equation



Adsorption isotherm of 17  $\beta$ -estradiol in water-methanol solution 98:2 % (m/m) at 288K, fitting with the Langmuir equations (—) and Freundlich equations (---).

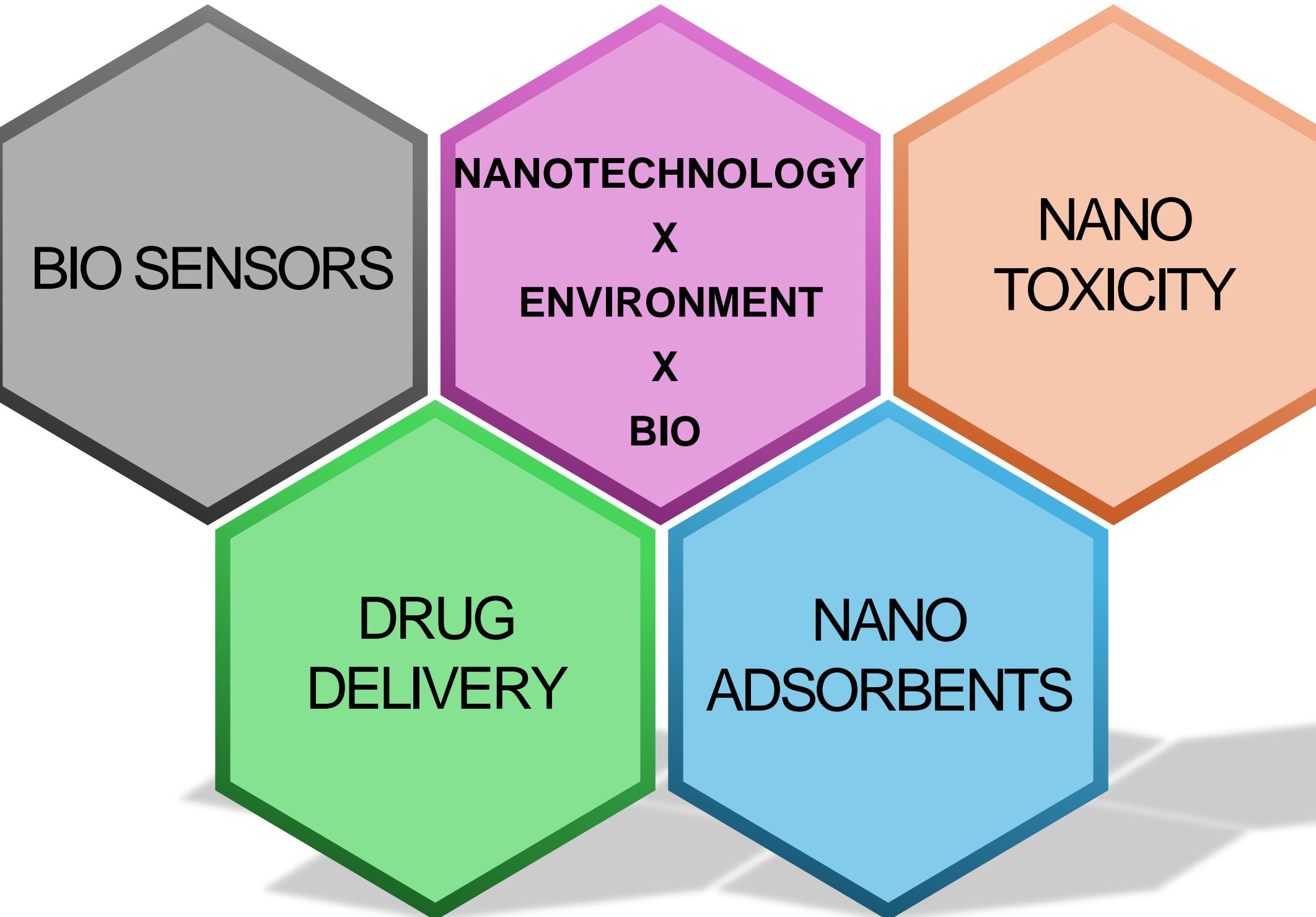
## COMPARATIVE RESULTS

Comparison of the maximum amount of adsorption of  $17\beta$ -estradiol in different nanomaterials.

Adsorbent material	$Q_{\max}$ (mg/g)	Treatment condition	Reference
GO, methanol	169.49	T=30°C	Present work
SWCNT	27.20	pH=7.5	Zaib et al., 2012[45]
Active carbon	21.3-67.6	pH=5	Fukuhara et al., 2006[46]
GO	48	T=25°C	Sun et al., 2017[47]
SM-NGO	106.38	T=30°C	Bai et al., 2017 [48]
Nanosheets of GO	149.4	T=25°C, pH=7	Jiang et al., 2016[49]
AMBCs-700	153.20	pH=6	Yin et al., 2018[50]
ATP/BC	154.23	pH=3.5	Yin et al., 2019[51]

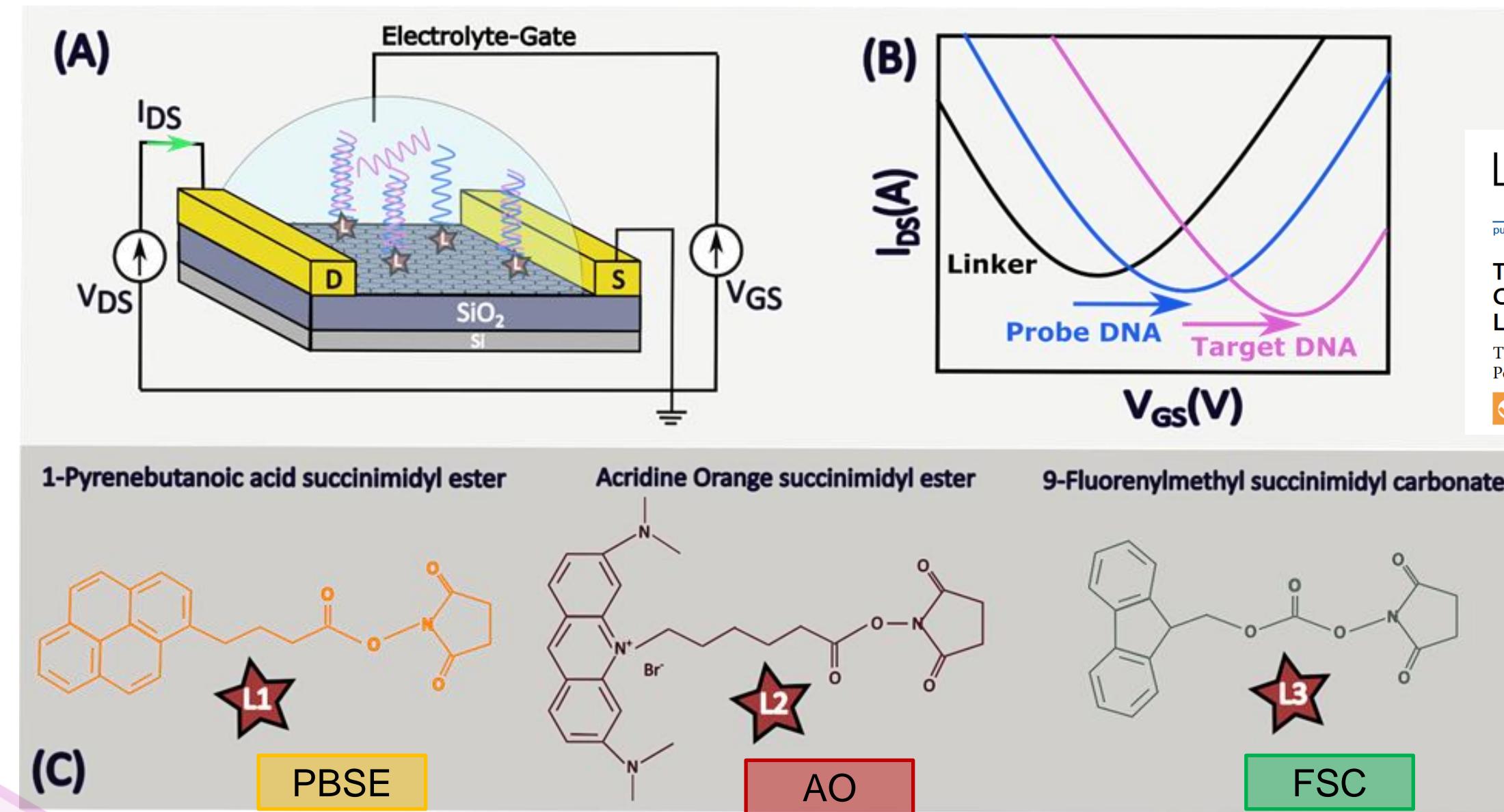
## CONCLUSIONS

- Adsorption capability of **graphene oxide (GO)** for removing **17 $\beta$ -estradiol** - proportions of water:methanol, 98:02, 90:10, 70:30 and 50:50% (m/m) and different temperatures, 288, 293, 318 and 328K.
- The *ab initio* investigation of the interaction of GO and 17 $\beta$ -estradiol showed most stable configuration with **energy of adsorption was 1.88 eV** when the molecule was under the **-COOH and -OH** functional groups in accordance with the FTIR experimental data.
- Methanol occupies active sites** of graphene oxide **reducing** the **surface area** for the endocrine disruptors and decreasing the 17 $\beta$ -estradiol adsorption.
- The **smaller concentration** of the co-solvent methanol (98:02% (m/m) of water:methanol at 288 K) provides an **increase of the 17 $\beta$ -estradiol adsorption** on the graphene oxide.
- WE SHOW ... innovative procedures to evaluate the ability of graphene oxide to remove endocrine disruptors from water using the synergy between experimental and *ab initio* results.**

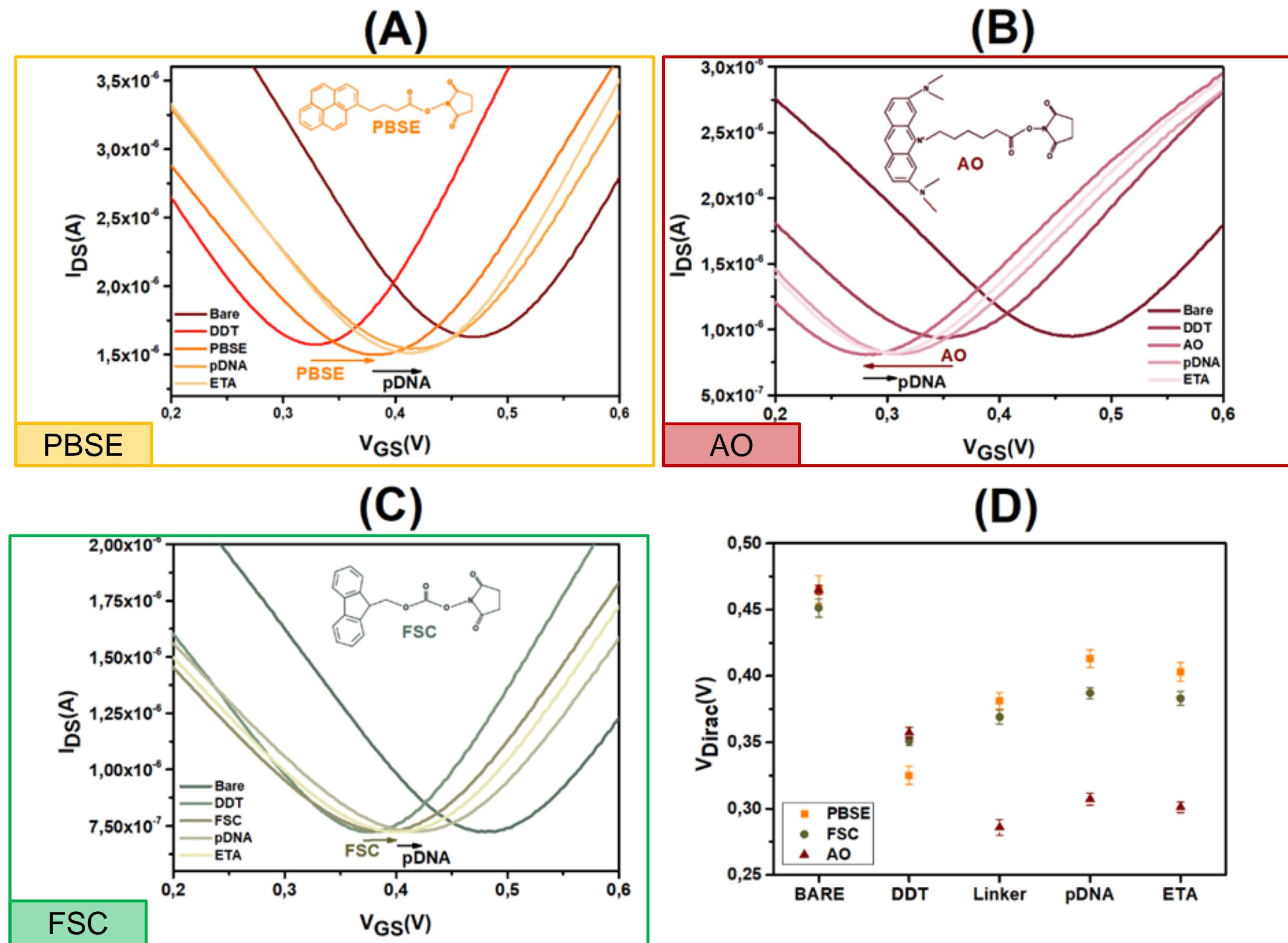


# DNA immobilization, binding kinetics, and hybridization efficiency on single-layer graphene through pyrene-, acridine- and fluorenyl methyl-based linkers

*Telma Domingues, João Rodrigues, M. Fátima Cerqueira, Joana Rafaela Guerreiro, Jérôme Borme, Mariana Zancan Tonel, Julia Schultz, Ivana Zanella da Silva, Solange Binotto Fagan, and Pedro Alpuim*



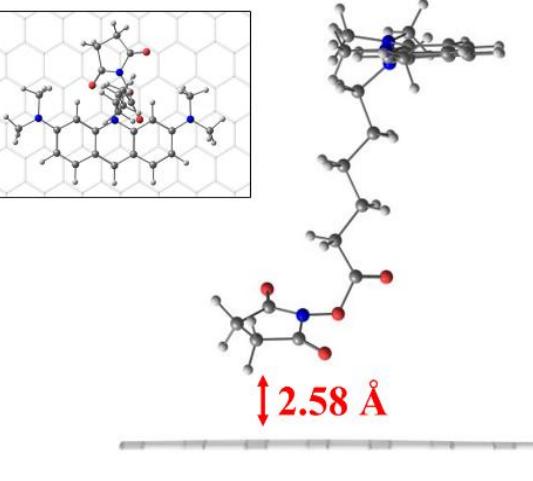
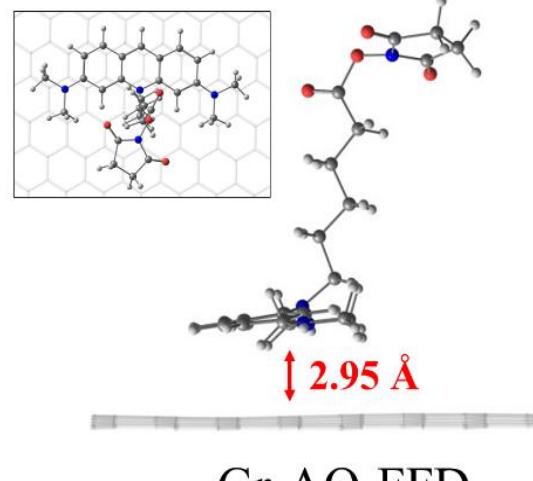
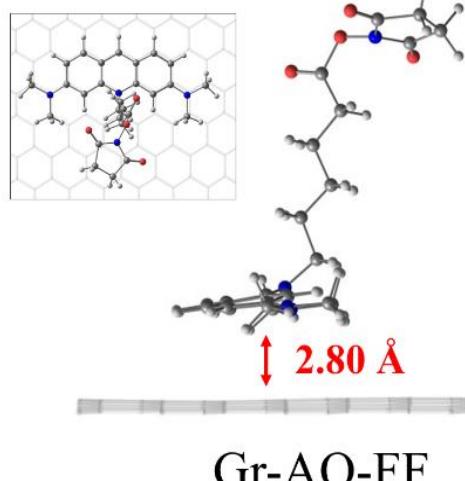
# EXPERIMENTAL RESULTS



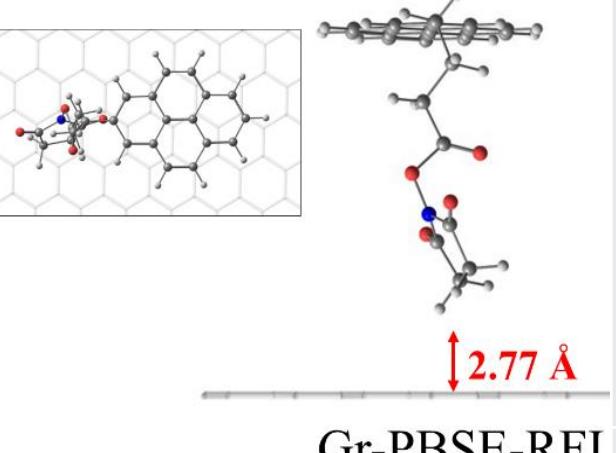
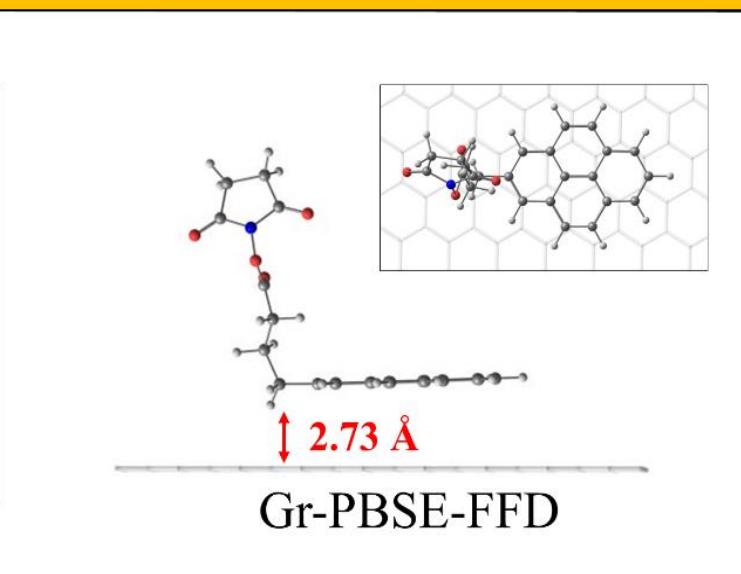
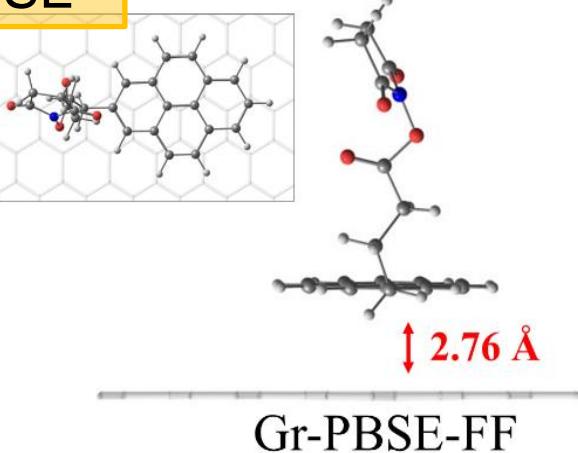
Graphene transistors transfer curves after each stage of graphene functionalization for the linkers: (A) PBSE, (B) AO, and (C) FSC. (D)  $V_{Dirac}$  for each step of graphene functionalization for each of the 3 linkers, PBSE (orange), AO (red) and FSC (green).

# ENERGETIC PROPERTIES

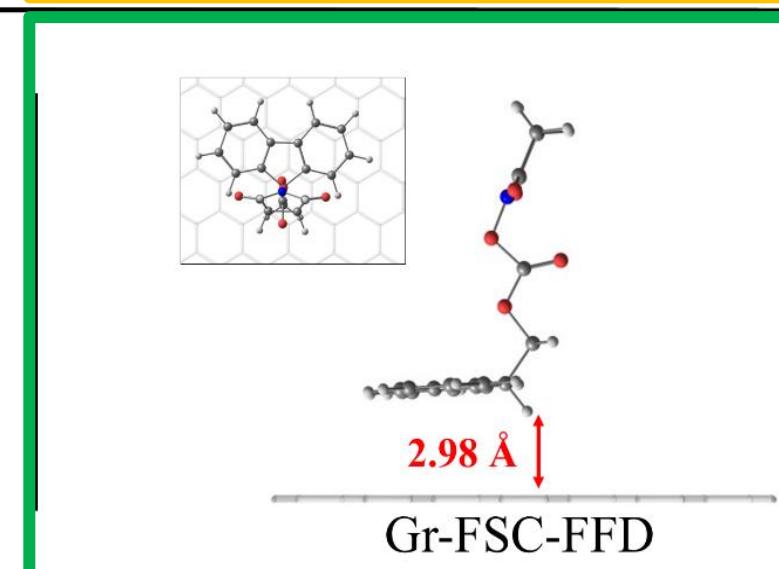
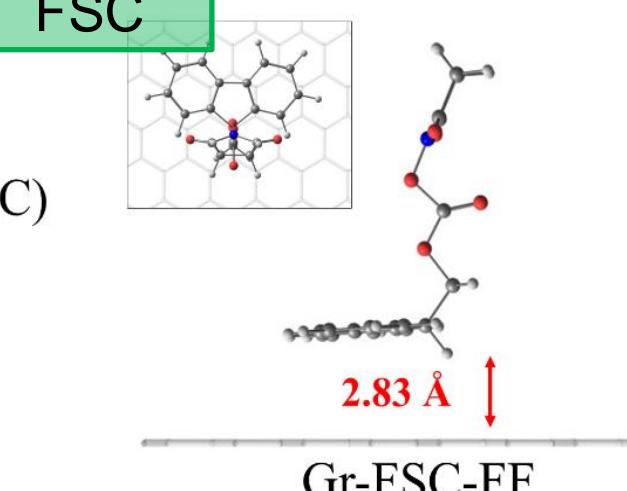
AO



PBSE



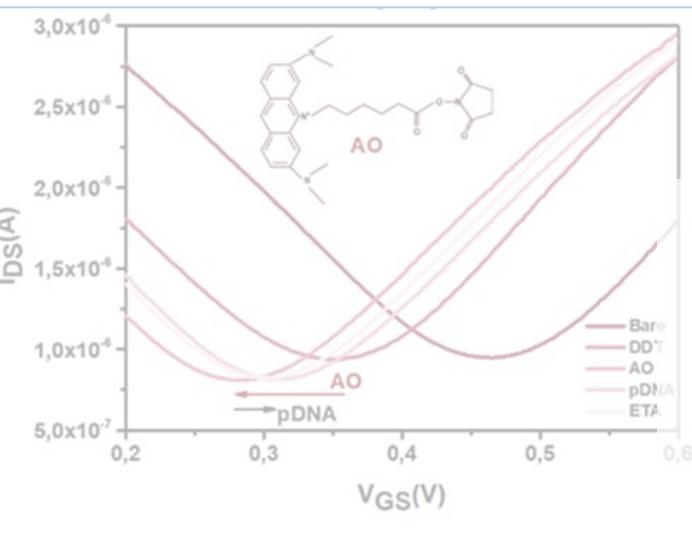
FSC



Configuration

	Configuration	Energy (eV)	Charge transfer (e <sup>-</sup> )	Distance (Å)
Gr-AO	FF	2.09	0.5	2.80 (C <sub>Gr</sub> - H <sub>AO</sub> )
	FFD	2.15	0.5	2.95 (C <sub>Gr</sub> - H <sub>AO</sub> )
	RFI	0.67	0.3	2.58 (C <sub>Gr</sub> - H <sub>AO</sub> )
Gr-PBSE	FF	1.19	-0.06	2.76 (C <sub>Gr</sub> - H <sub>PBSE</sub> )
	FFD	1.20	-0.06	2.73 (C <sub>Gr</sub> - H <sub>PBSE</sub> )
	RFI	0.27	-0.04	2.77 (C <sub>Gr</sub> - H <sub>PBSE</sub> )
Gr-FSC	FF	0.93	-0.04	2.83 (C <sub>Gr</sub> - H <sub>FSC</sub> )
	FFD	0.94	-0.05	2.98 (C <sub>Gr</sub> - H <sub>FSC</sub> )
	RFI	0.29	-0.04	3.06 (C <sub>Gr</sub> - H <sub>FSC</sub> )

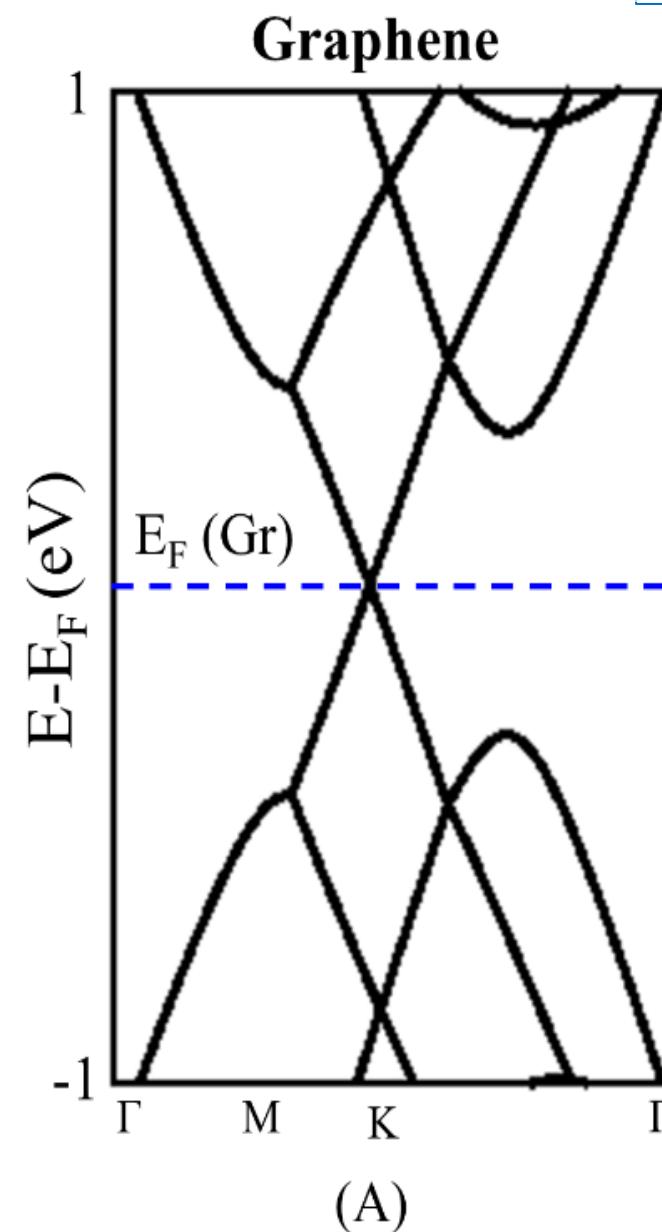
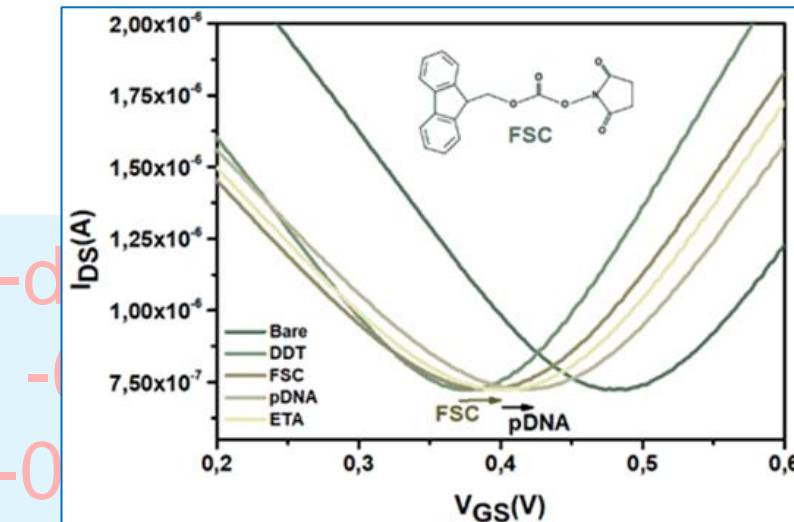
# ELECTRONIC PROPERTIES



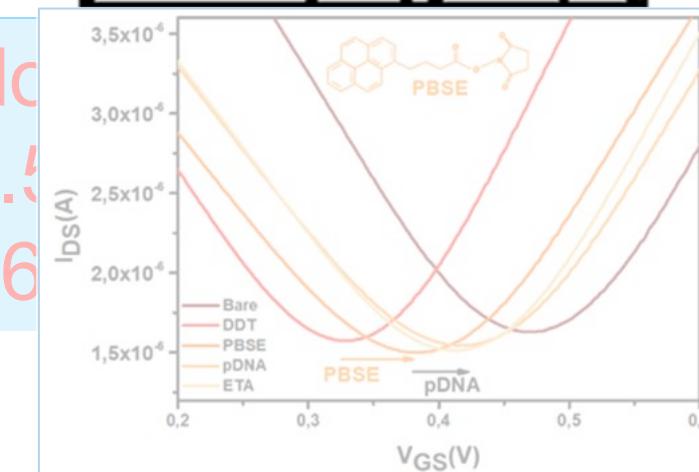
# Graphene as p-doped

## $\Delta\text{charge} = -0.01$

## $\Delta\text{Dirac} = -0.01$



# Graphene as n-dc $\Delta_{\text{charge}} = 0.5$ $\Delta_{\text{Dirac}} = 0.6$



# Graphene as p-doping

$\Delta\text{charge} = -0.05 \text{ e-}$

$\Delta\text{Dirac} = -0.06 \text{ eV}$

# DNA immobilization, binding kinetics, and hybridization efficiency on single-layer graphene through pyrene-, acridine- and fluorenyl methyl-based linkers

*Telma Domingues, João Rodrigues, M. Fátima Cerqueira, Joana Rafaela Guerreiro, Jérôme Borme, Mariana Zancan Tonel, Julia Schultz, Ivana Zanella da Silva, Solange Binotto Fagan, and Pedro Alpuim*

- Theoretical *ab initio* analyses further elucidated the interaction mechanisms between pristine graphene and the linkers **AO, PBSE, and FSC**.
- The **van der Waals binding energy** and electronic band structure confirmed **stable interactions of the biofunctional linkers adsorbed on the graphene**.
- Mulliken population analysis identified ambipolar charge transfer effects, where AO acted as an electron acceptor (**graphene n-doping**) and PBSE and FSC functioned as electron donors (**graphene p-doping**).
- Experimental and theoretical insights provide a comprehensive understanding of the physical and chemical behavior of the functionalized nanosystem, paving the way for future advancements in biosensor development.

*Langmuir* > Vol 41/Issue 29 > Article

ARTICLE | July 20, 2025

**Graphene Surface Functionalization with Pyrene-, Acridine-, and Fluorenyl-Linkers for DNA Hybridization Studies Using Electrolyte-Gate Graphene Field Effect Transistors**

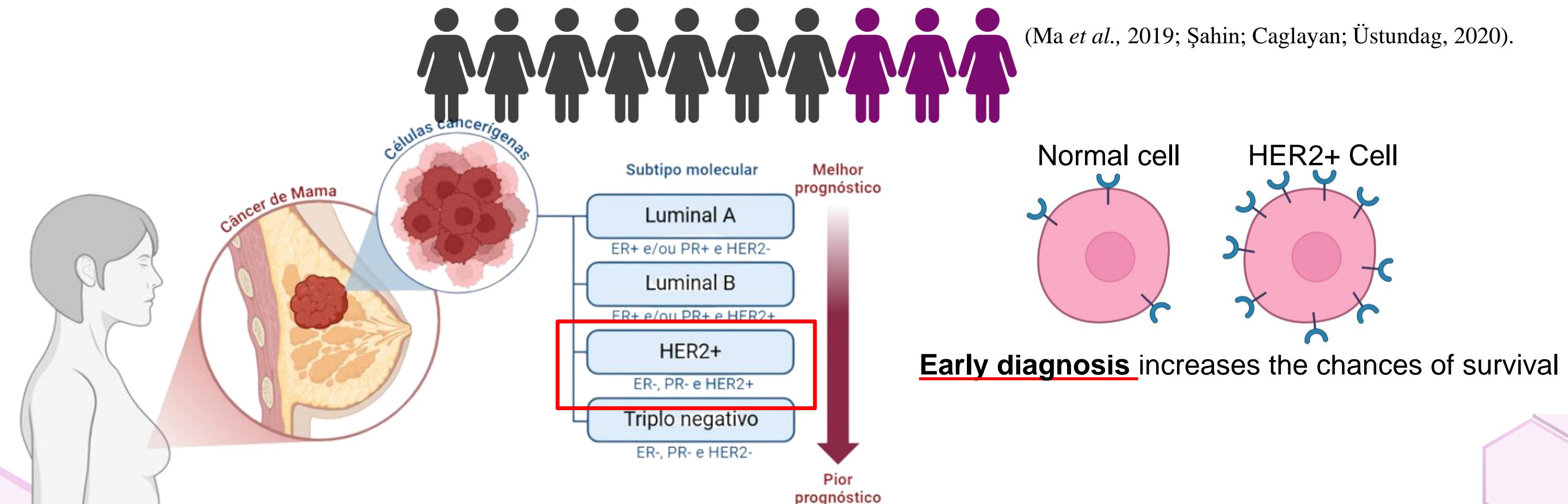
Telma Domingues\*, , João Rodrigues, , M. Fátima Cerqueira, , Joana Rafaela Guerreiro, , Jérôme Borme, , Mariana Zancan Tonel, , Julia Schultz, , Ivana Zanella, , Solange Binotto Fagan, , and , Pedro Alpuim\*

Cite Share Jump to Expand

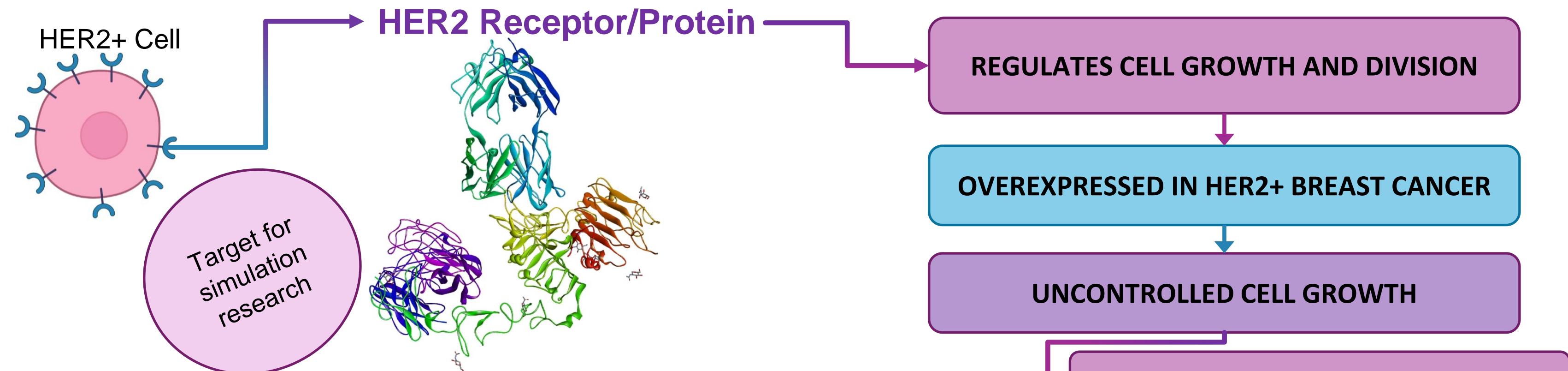
# GFET(graphene field-effect transistors) biofunctionalization through pyrene-methyl-based linker to detect the breast cancer biomarker HER2 protein

*Julia Schultz, Telma Domingues, M. Fátima Cerqueira, Jérôme Borme, Mariana Zancan Tonel, Ivana Zanella da Silva, Solange Binotto Fagan, and Pedro Alpuim*

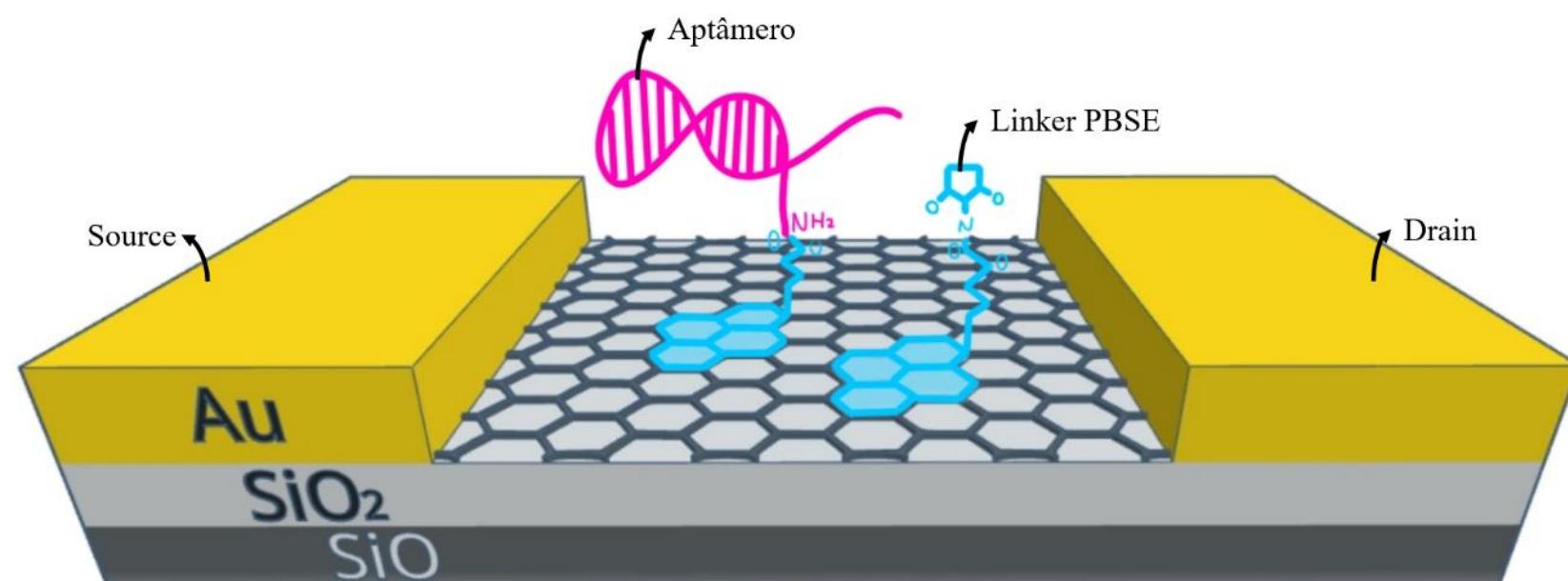
**20 to 30% of BC cases are diagnosed as HER2+**  
(Human Epidermal Growth Factor Receptor type 2)



# GFET biofunctionalization through pyrene-methyl-based linker to detect the breast cancer biomarker HER2 protein



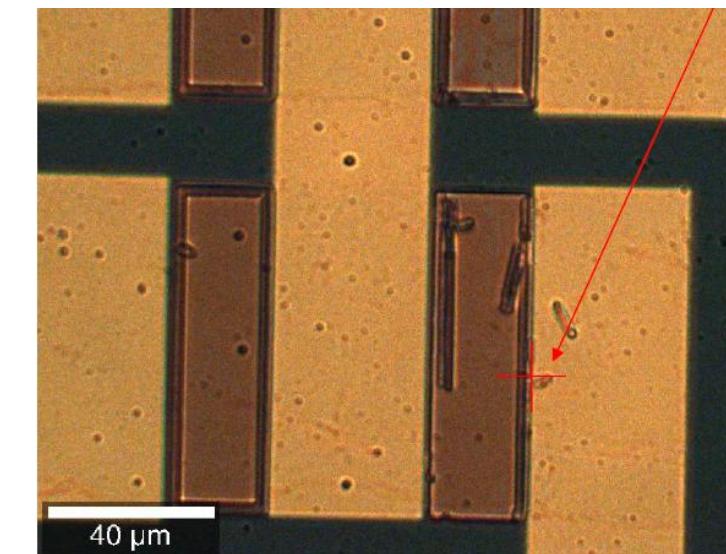
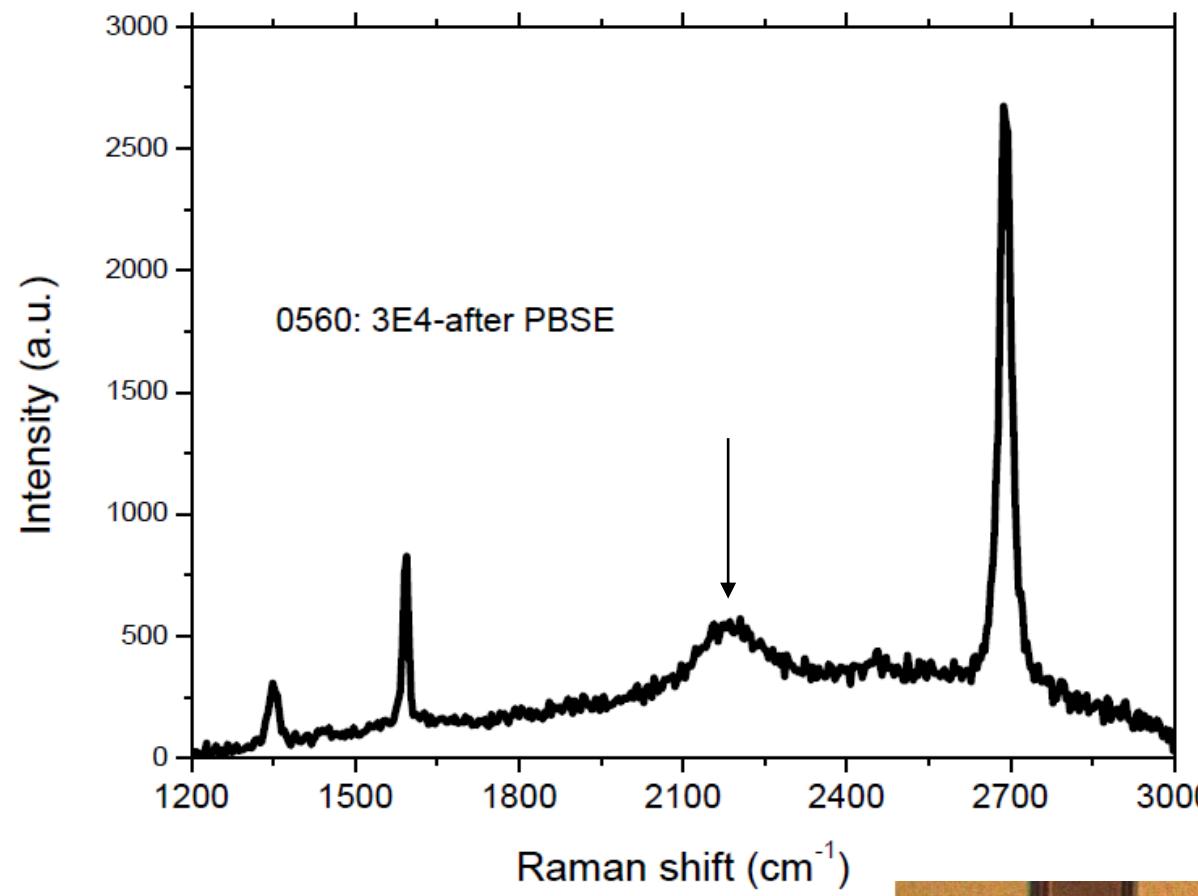
## Functionalized GFET as a HER2 protein detector



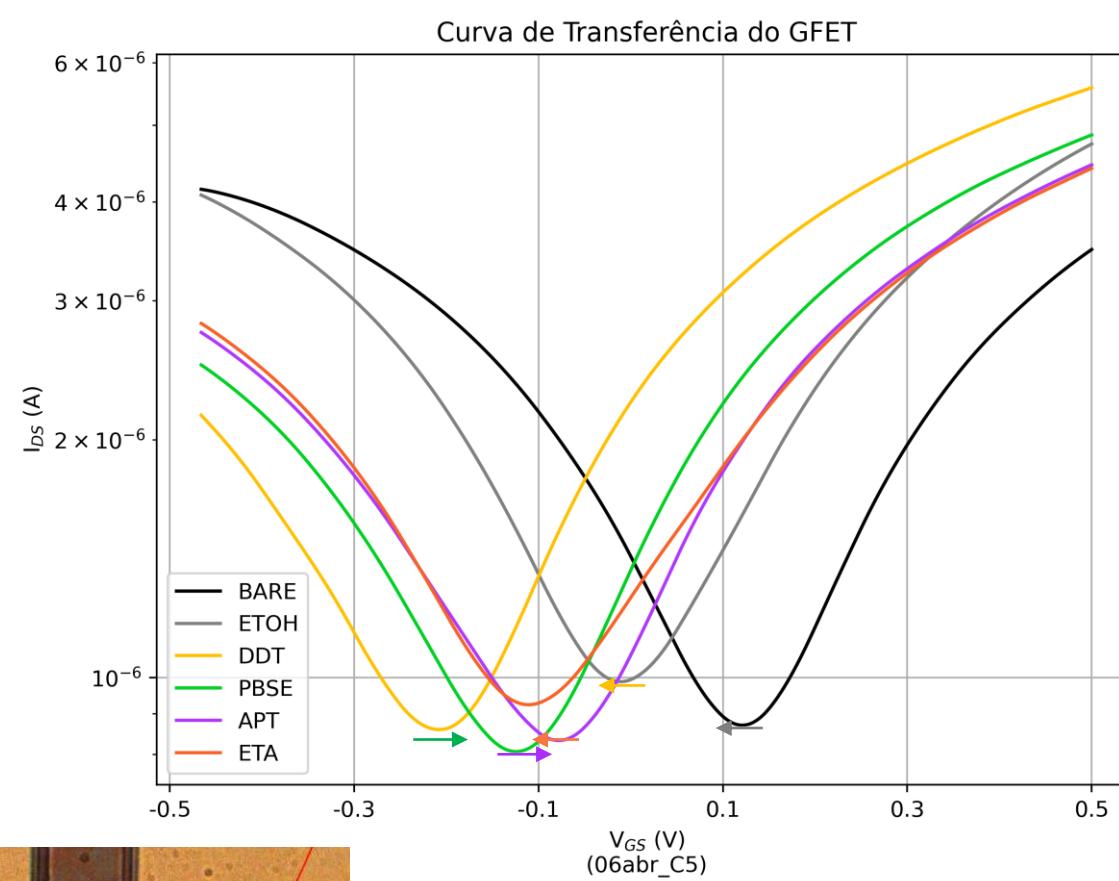
THE BC IS MORE AGGRESSIVE AND HAS POOR PROGNOSTICS, EARLY DIAGNOSIS IS ESSENTIAL

# GFET biofunctionalization through pyrene-methyl-based linker to detect the breast cancer biomarker HER2 protein

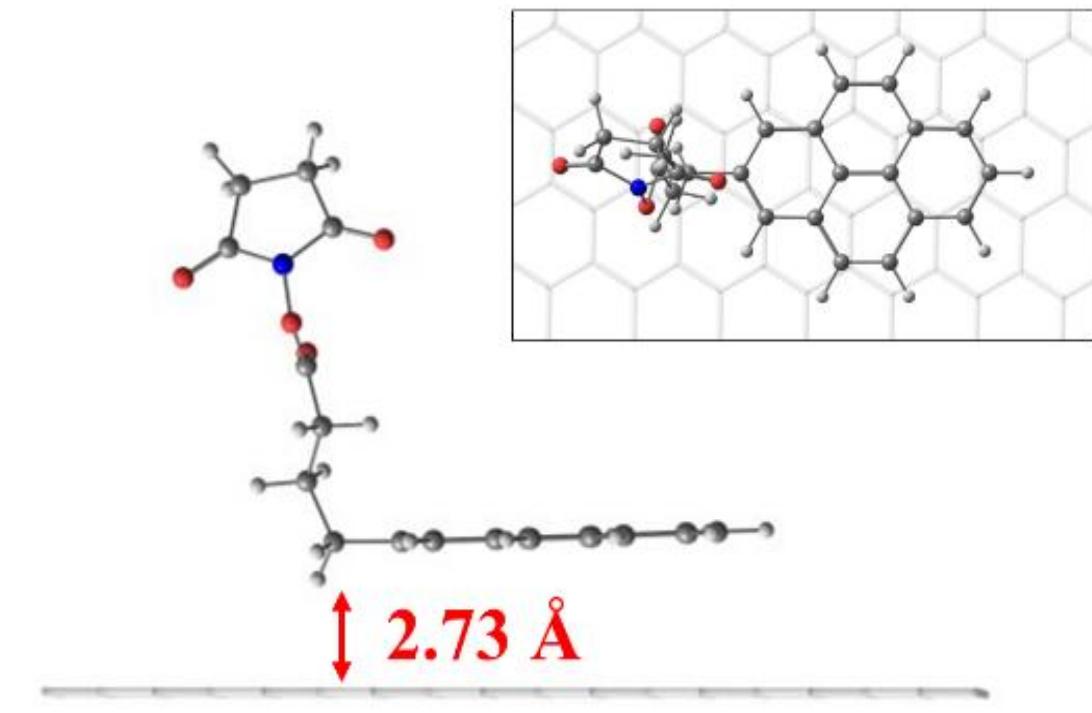
## Characterization



## Linker functionalization Experimental



## Theoretical/Simulation

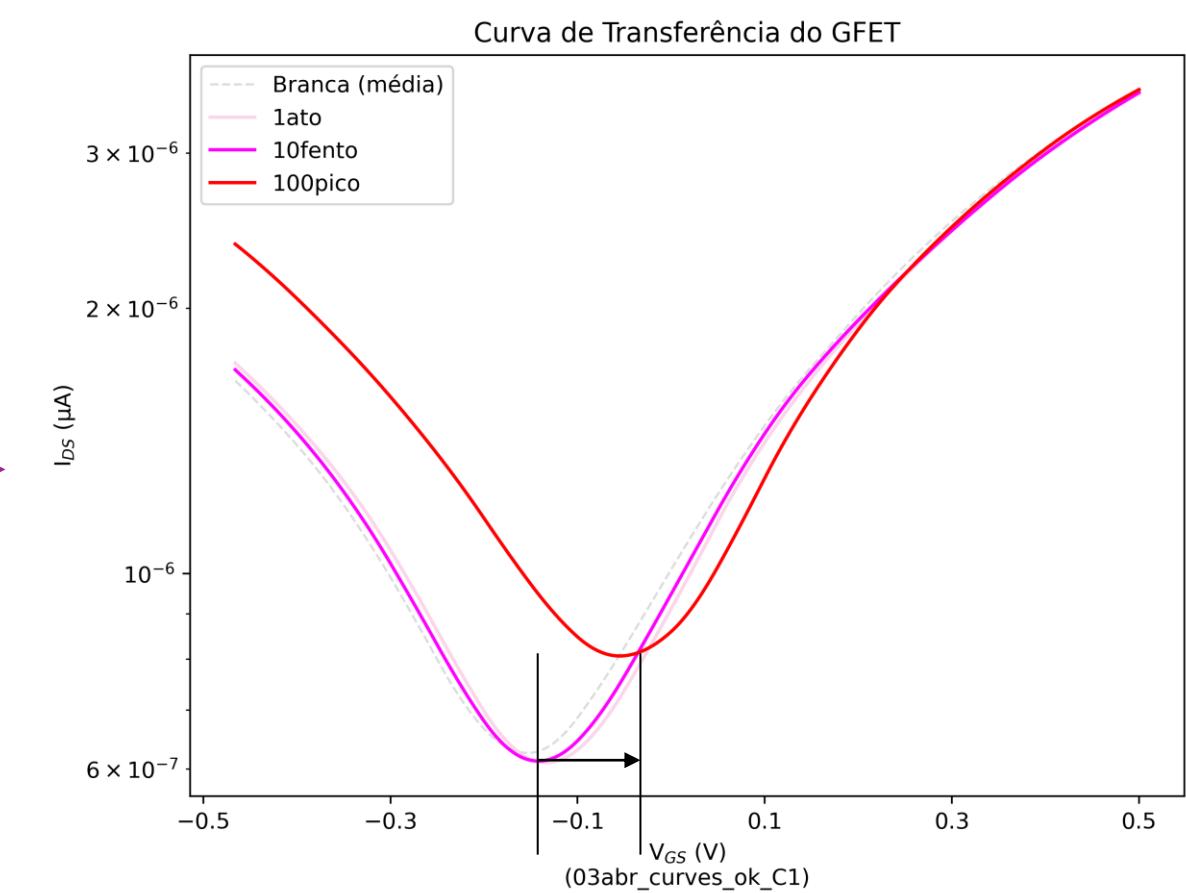


Gr-PBSE-FFD

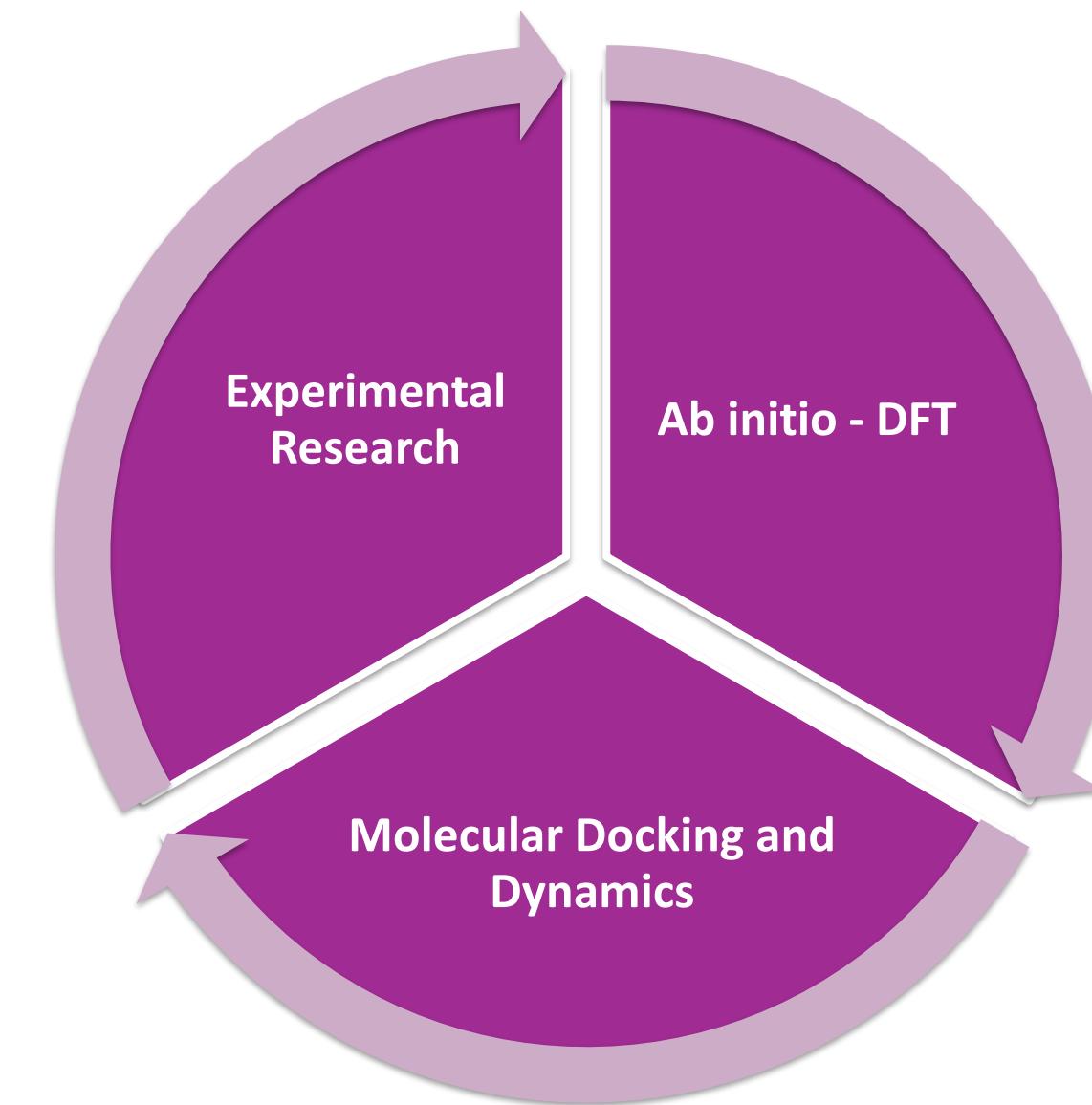
Energy (eV)	Charge transfer (e⁻)
1.20	0.06

# GFET biofunctionalization through pyrene-methyl-based linker to detect the breast cancer biomarker HER2 protein

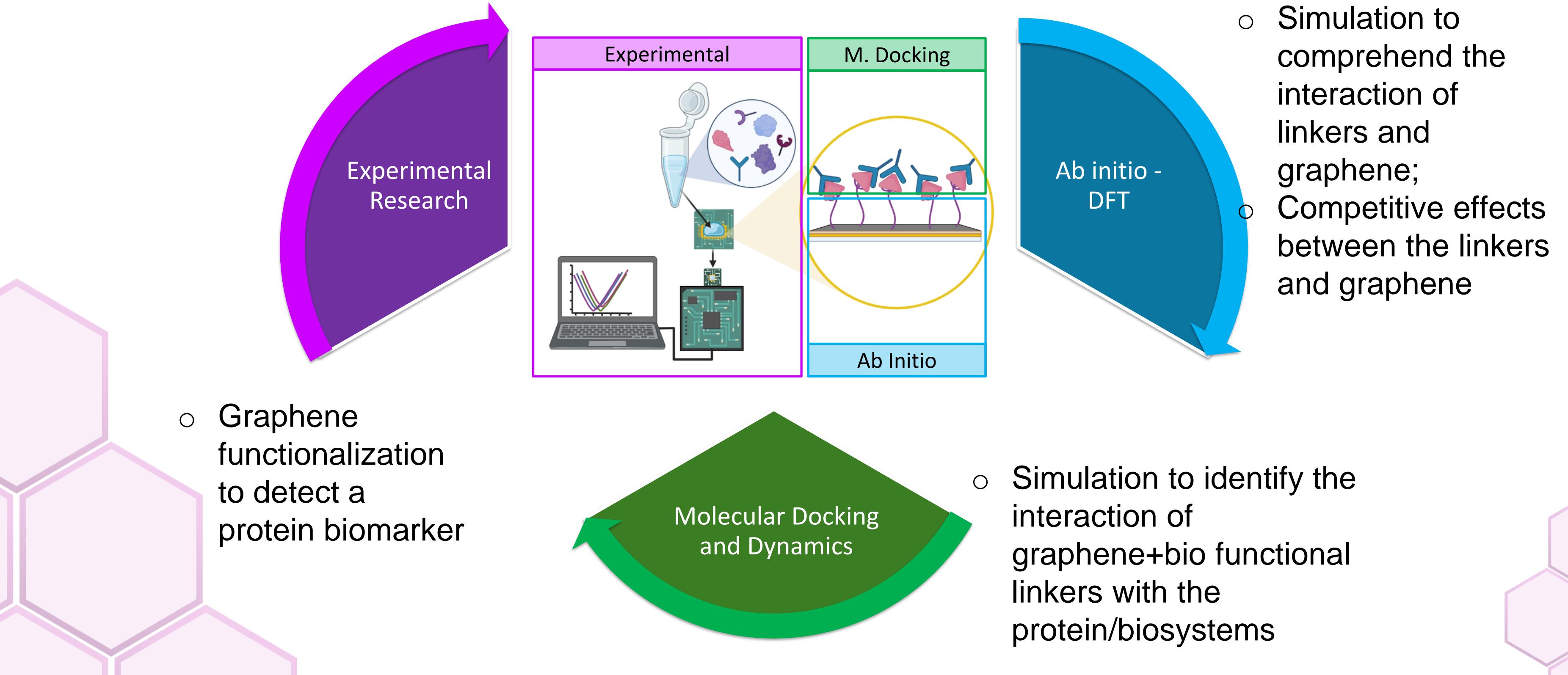
- Experimental results and characterization via Raman spectroscopy confirm the presence of graphene in GFET and its functionalization with the PBSE linker;
- The experimental results show the success of the methodology for functionalizing graphene in GFETs for anchoring aptamers;
- The chosen aptamer is specific for binding to the HER2 protein according to literature data;
- Experimental studies indicated variation between blank (without protein) and positive (with HER2 protein) samples;
  - The next steps of the research are to analyze, via computer simulation (docking molecular and molecular dynamics):
    - The interaction and competitiveness between linkers with graphene
    - The linker-aptamer interaction
    - The aptamer-protein interaction



# THEORETICAL STUDY OF LINKERS ADSORPTION ON PRISTINE GRAPHENE FOR BIOSENSING APPLICATIONS



# THEORETICAL STUDY OF LINKERS ADSORPTION ON PRISTINE GRAPHENE FOR BIOSENSING APPLICATIONS

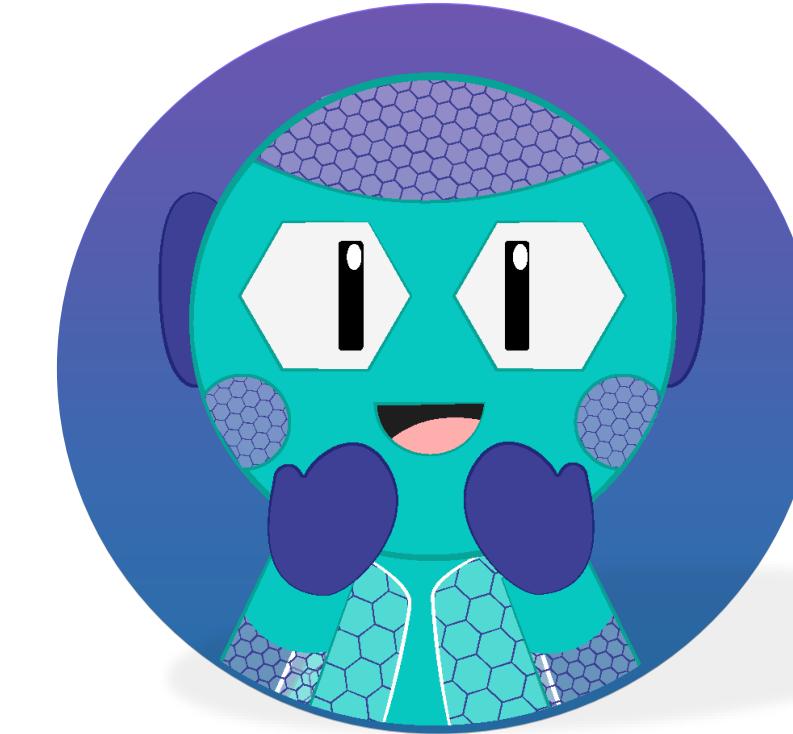




# Outreach and (Nano)Science Dissemination



Brazilian Network of  
Woman in  
Nanoscience



The Wonderful Nanometric  
World



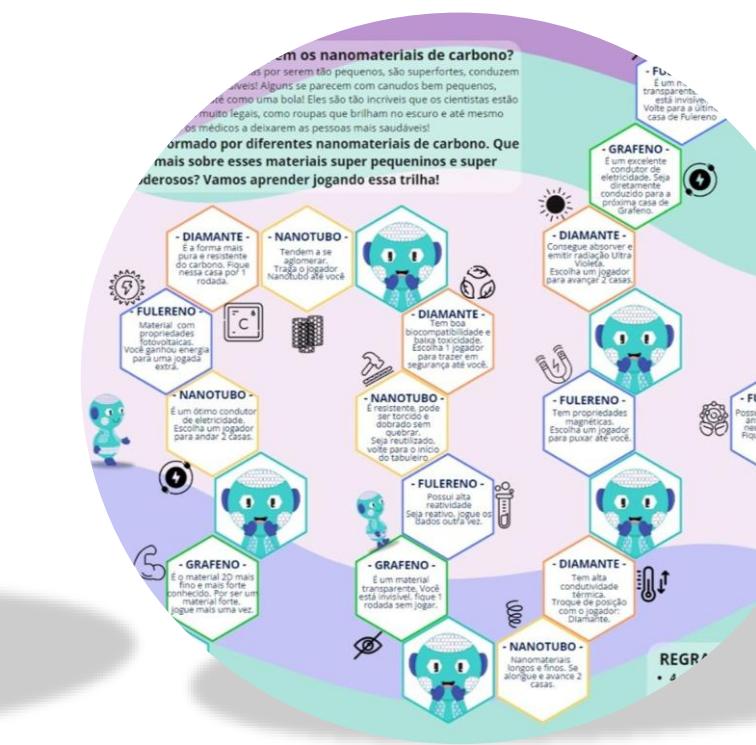
MBA Course  
EAD



Short Courses  
EAD



Virtual Reality in Nano



Board Game



Nano Games

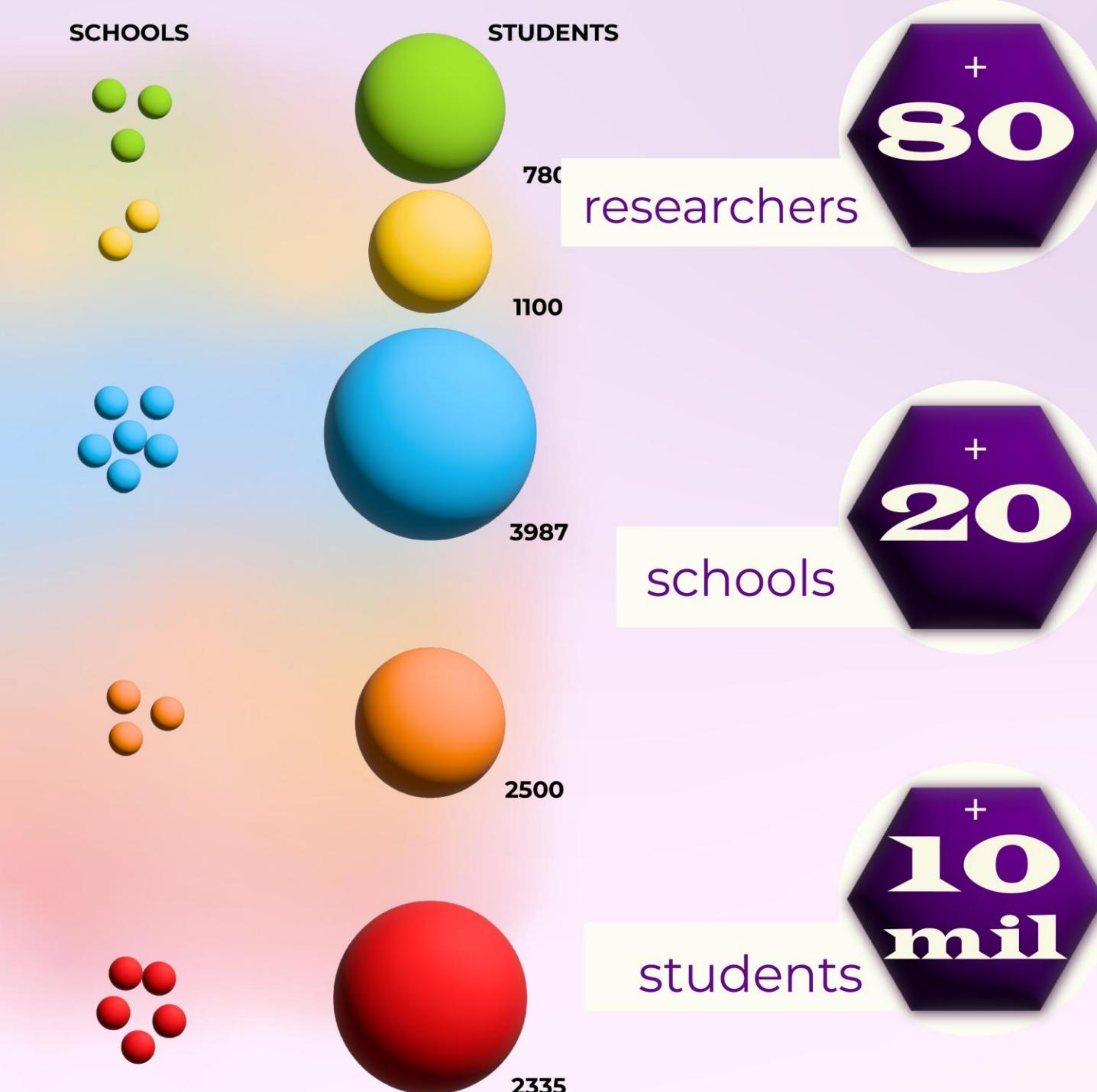
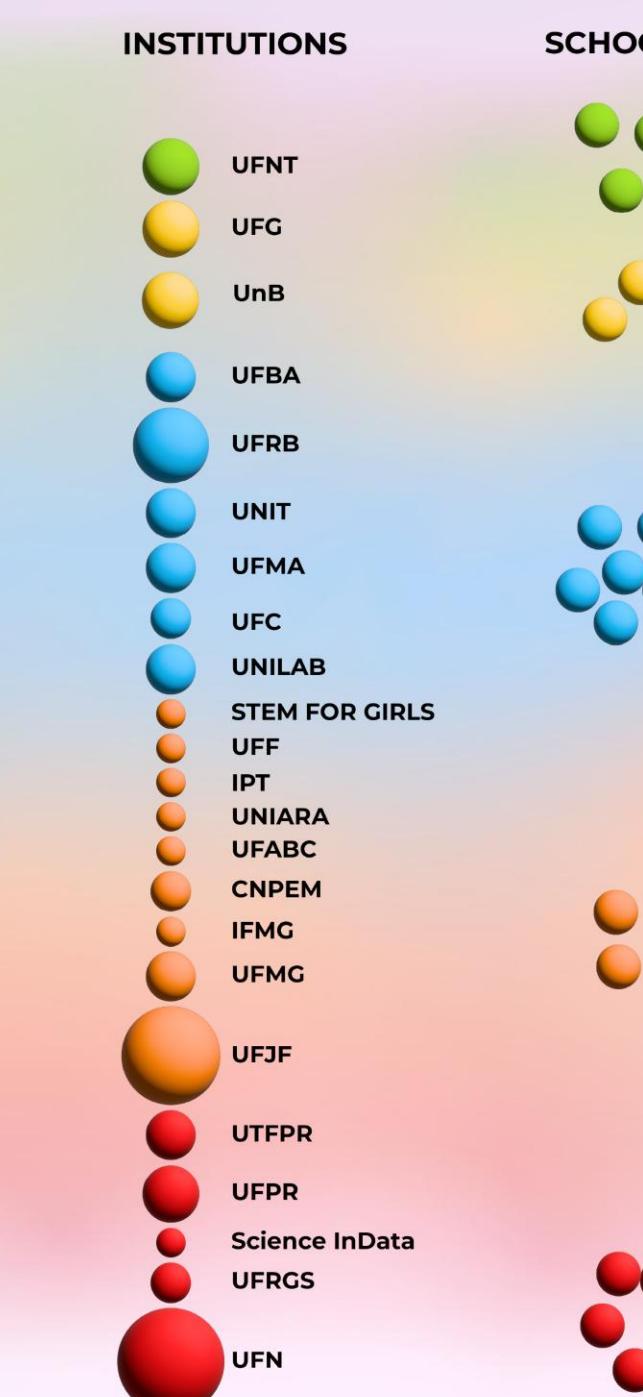
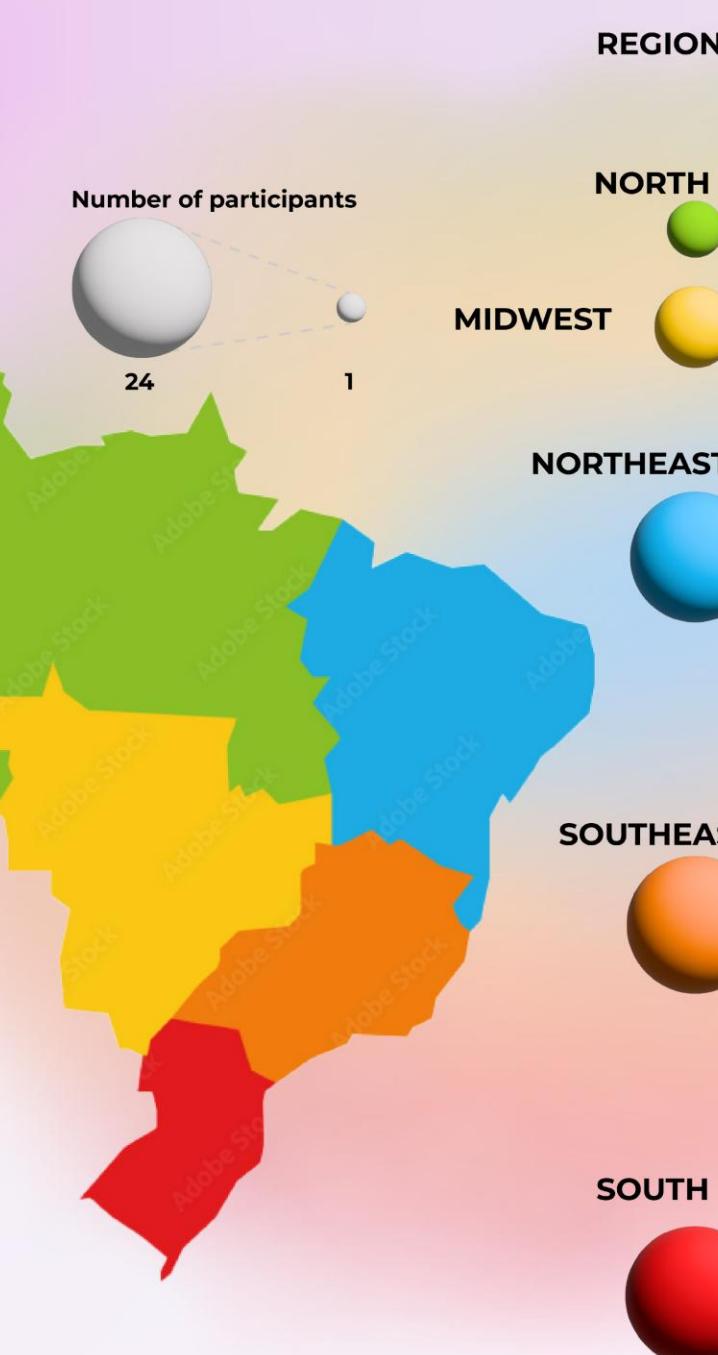


Book



# Women in Nanoscience

*Knowledge and Innovation for  
Scientists and Professionals of the Future*



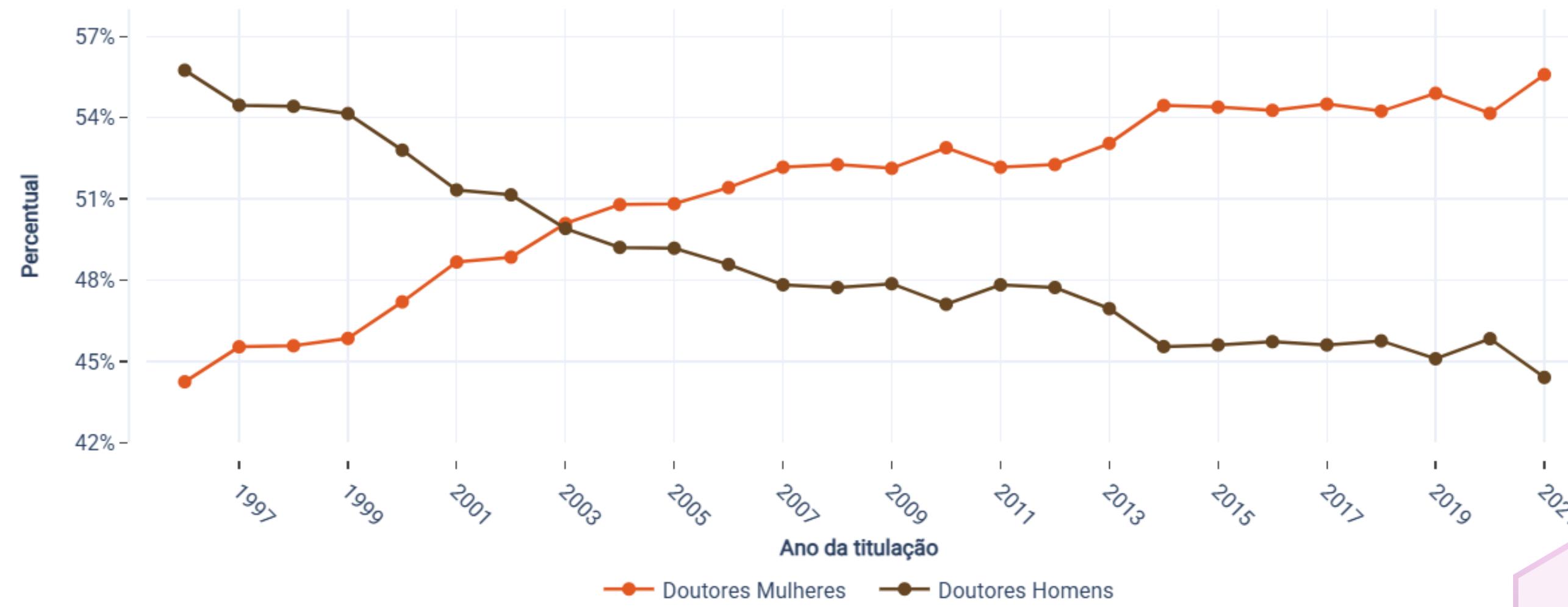


## Por que uma Rede de Mulheres na Nanociência?

Mestres Doutores



Proporção de mulheres e homens entre os titulados, 1996-2021 (%)



Fonte: Elaboração do CGEE a partir de dados da Plataforma Sucupira - Capes/MEC (1996-2021). Tabelas M.TIT.11 e D.TIT.11

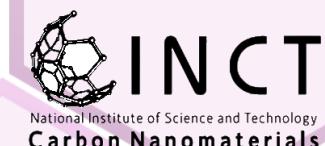




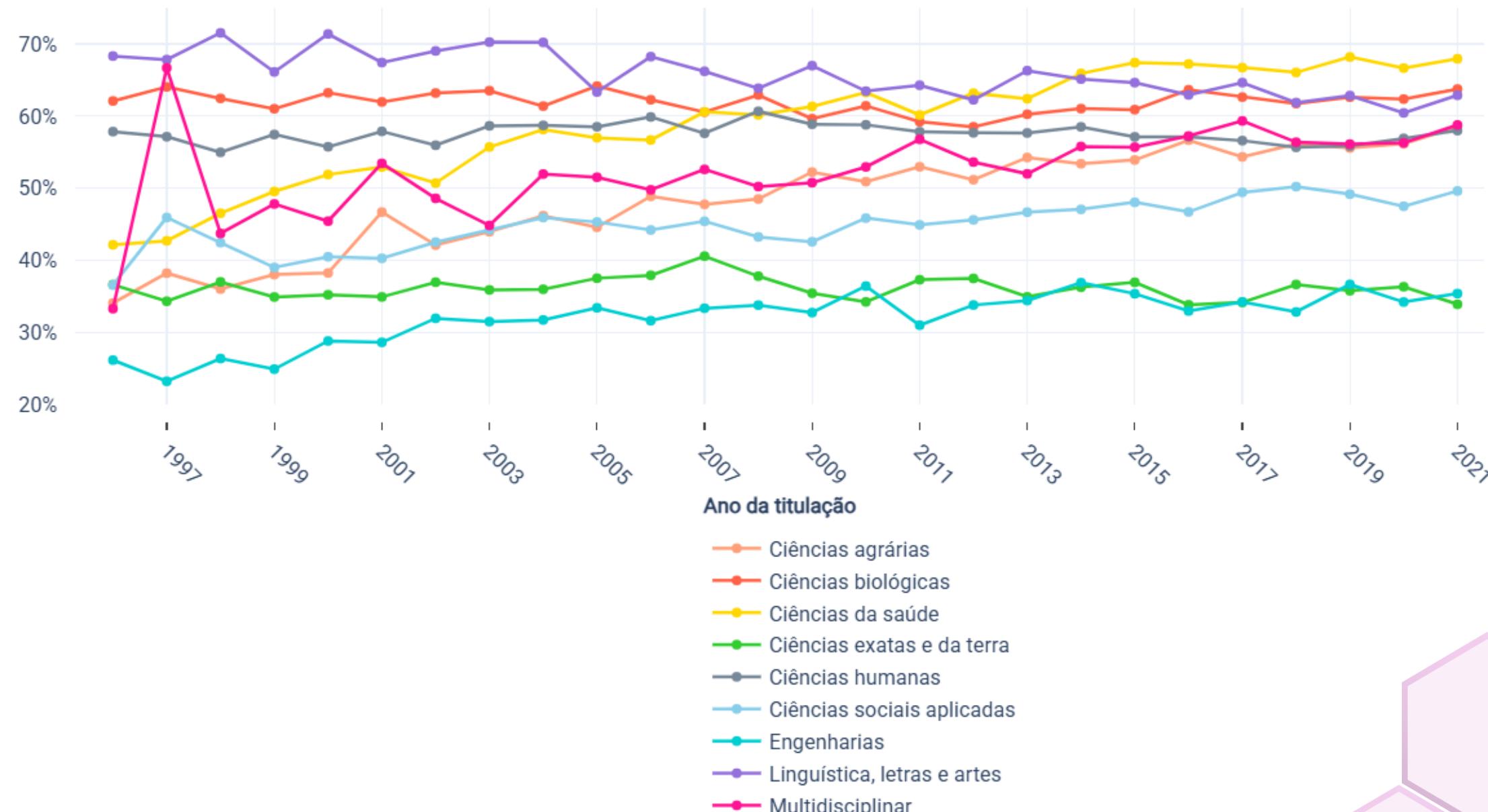
Gráfico 5.3.1

## Por que uma Rede de Mulheres na Nanociência?

Mestres Doutores



Participação de mulheres entre os titulados por grande área do conhecimento, 1996-2021 (%)



Fonte: Elaboração do CGEE a partir de dados da Plataforma Sucupira - Capes/MEC (1996-2021). Tabelas M.TIT.05 e D.TIT.05





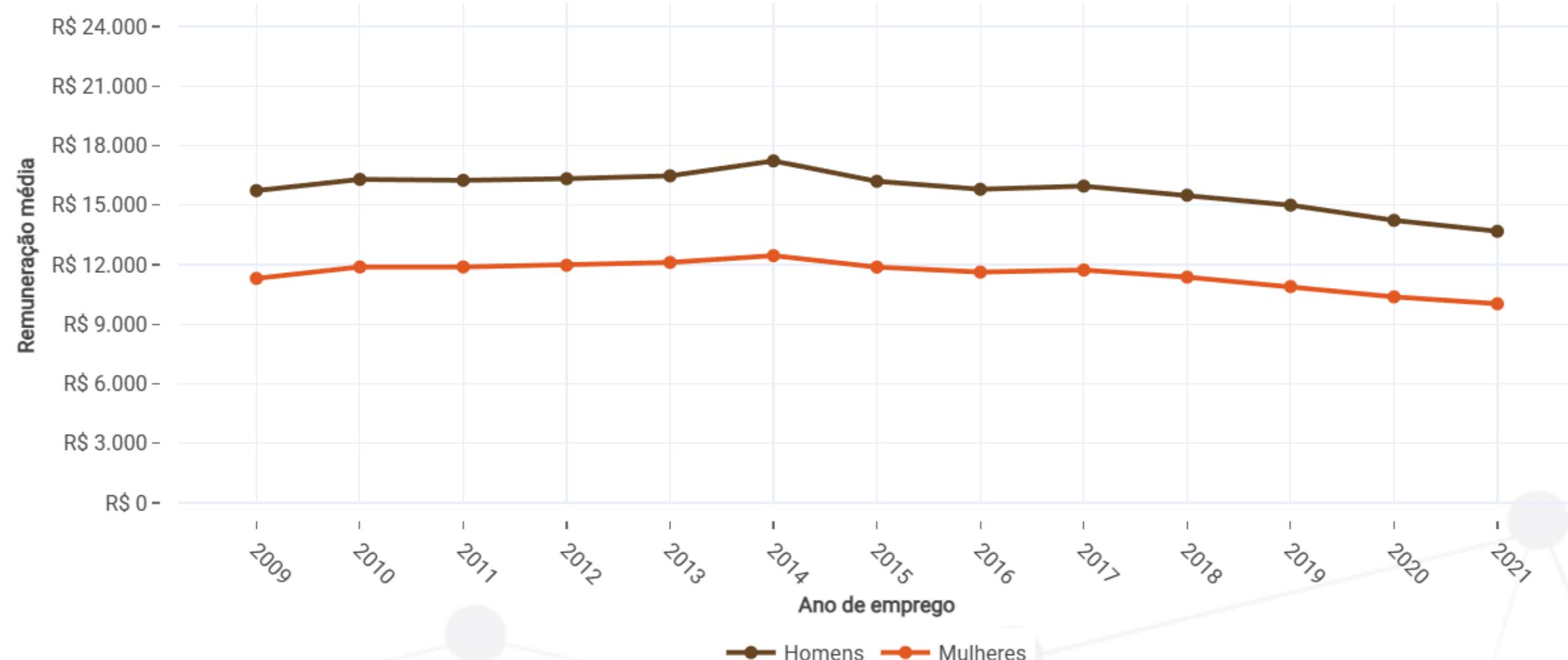
## Por que uma Rede de Mulheres na Nanociência?

Gráfico 5.5.1

Mestres Doutores



Remuneração mensal média de mulheres e homens no Brasil, 2009-2021 (R\$ constantes de 12/2021)



Fonte: Elaboração CGEE a partir de dados da Plataforma Sucupira - Capes/MEC (1996-2021) e RAIS/MTE (2009-2021). Tabelas M.REM.02 e D.REM.02

Nota: O gráfico 5.5.1 apresentado acima é idêntico ao gráfico 7.8.1, que se encontra no capítulo 7 dedicado à remuneração.



## Por que uma Rede de Mulheres na Nanociência?

Gráfico 5.6.1



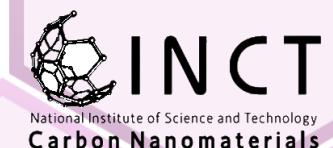
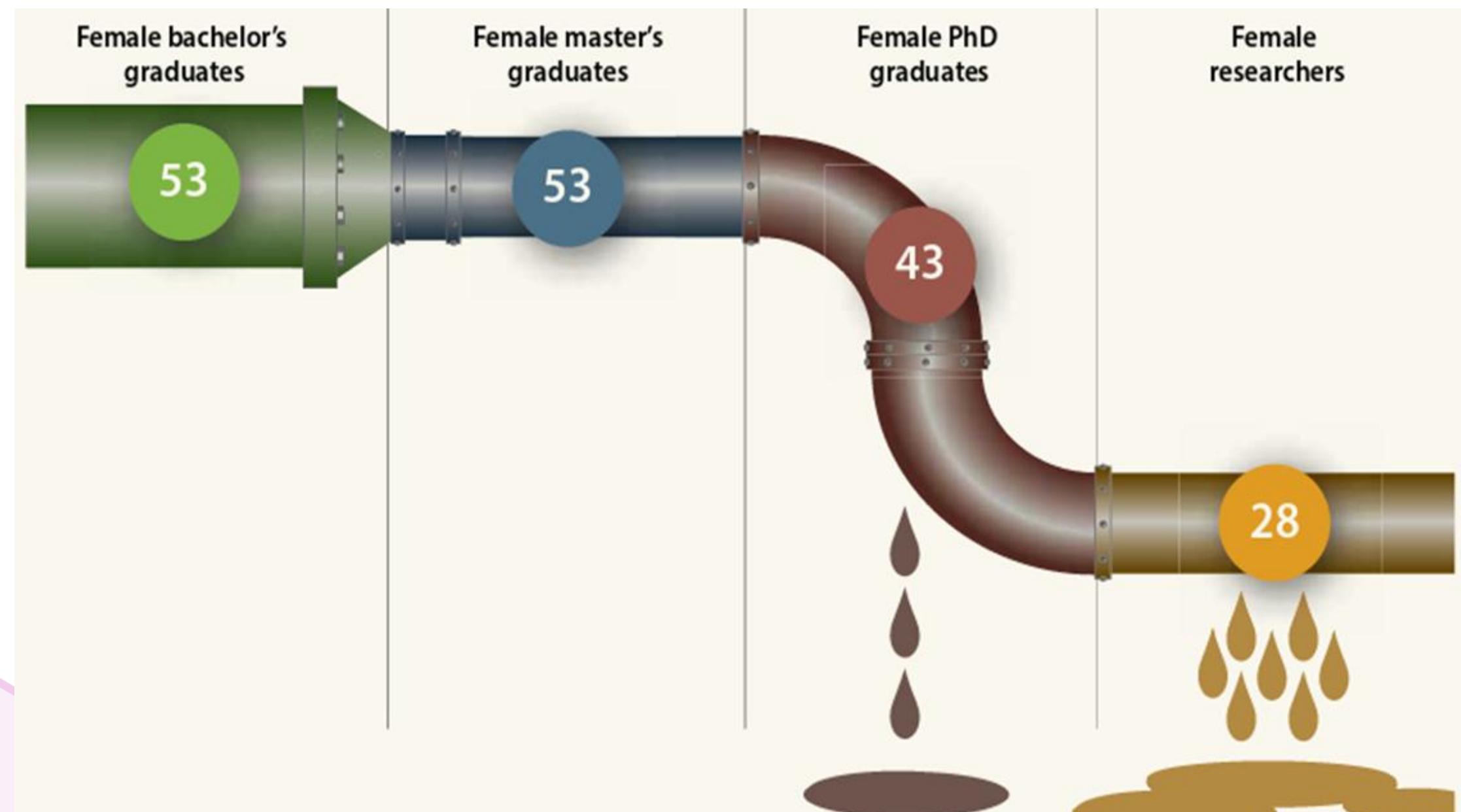
Mestres e doutores: Diferença entre a remuneração mensal média de mulheres em relação à dos homens por grande área do conhecimento, 2021 (%)



Fonte: Elaboração CGEE a partir de dados da Plataforma Sucupira - Capes/MEC (1996-2021) e RAIS/MTE (2021). Tabelas M.REM.09 e D.EMP.09



## Por que uma Rede de Mulheres na Nanociênci



UNESCO SCIENCE REPORT (2015)



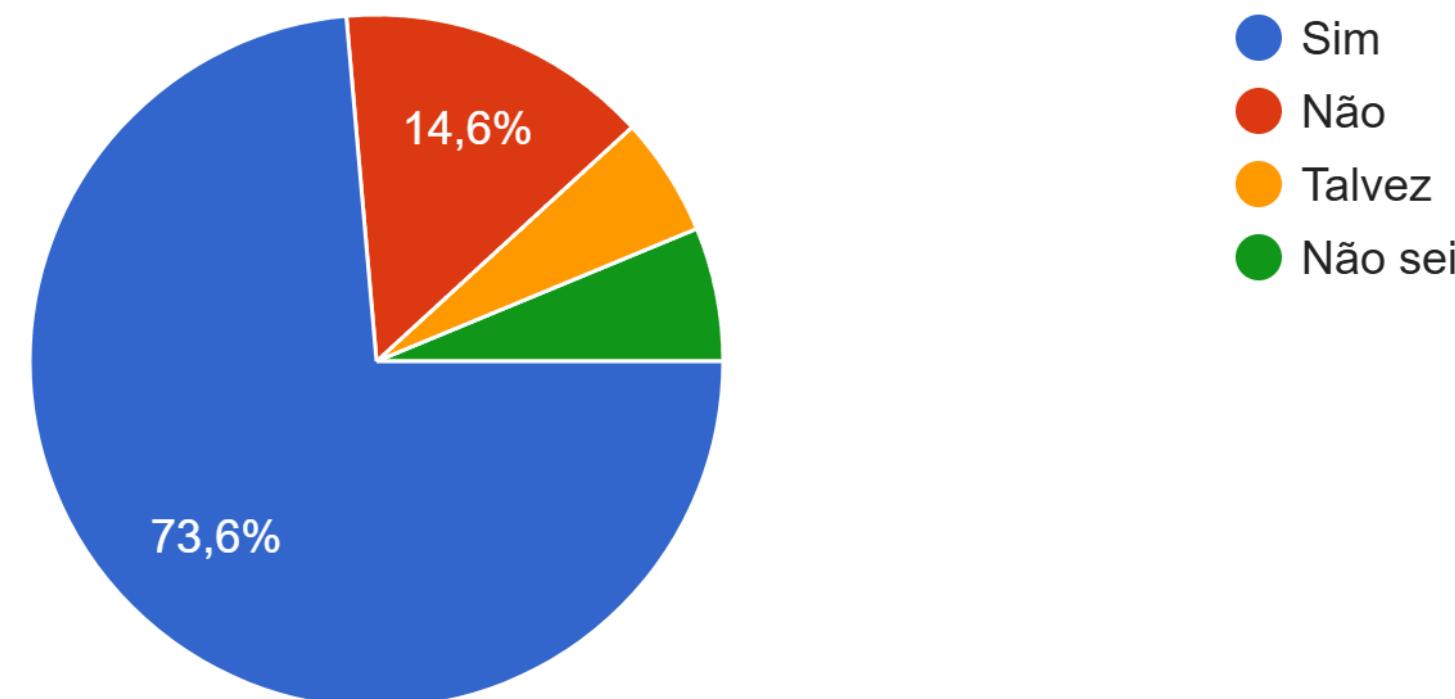
## Panorama das Mulheres Pesquisadoras e Empreendedoras em Nanociências no Brasil

Este formulário faz parte do projeto **Rede de Mulheres na Nanociência (CNPq)** (*Parecer do Comitê de Ética 78928224.8.0000.5306*).



Você já se sentiu pressionada a adiar ou evitar ter filhos por receio de impactar sua carreira acadêmica/profissional?

144 respostas





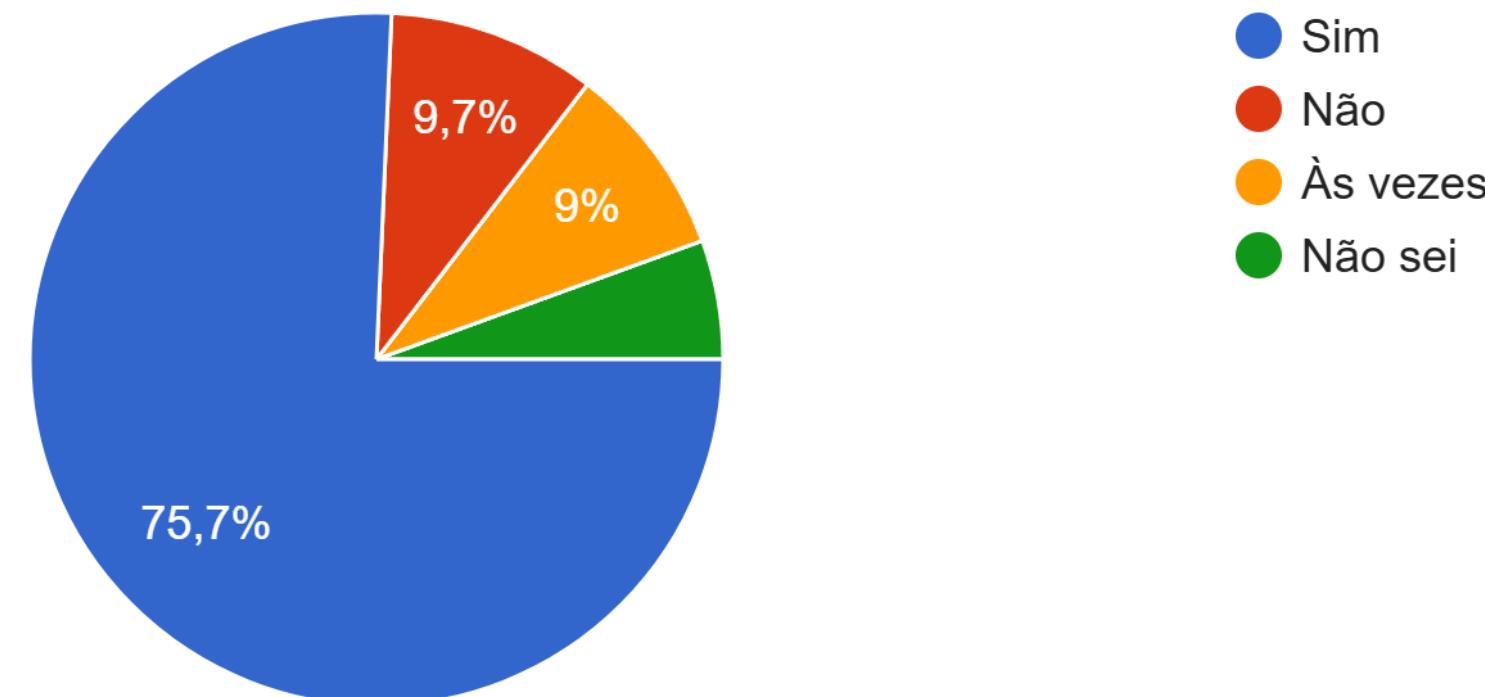
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Este formulário faz parte do projeto **Rede de Mulheres na Nanociência (CNPq)** (*Parecer do Comitê de Ética 78928224.8.0000.5306*).



Você já sentiu que seus colegas homens tiveram mais oportunidades ou reconhecimento no seu campo por causa do seu gênero?

144 respostas





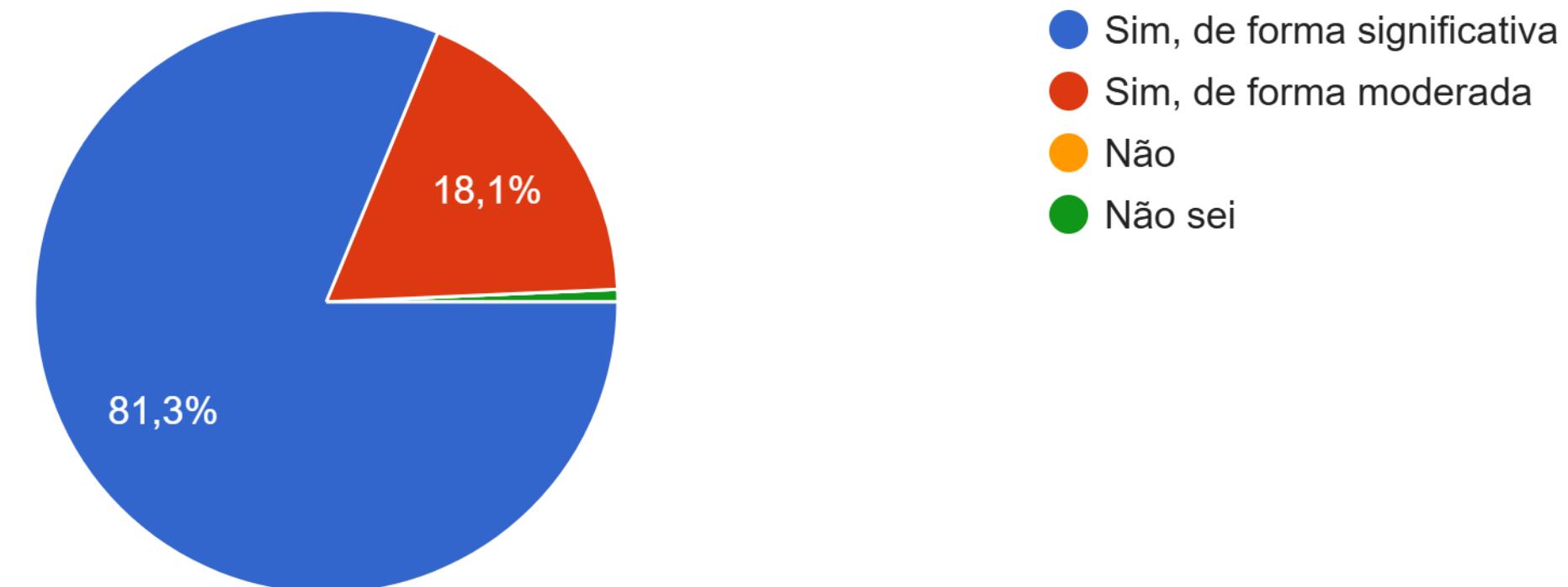
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Este formulário faz parte do projeto **Rede de Mulheres na Nanociência** (CNPq) (*Parecer do Comitê de Ética 78928224.8.0000.5306*).



Você acha que a visibilidade das mulheres na N&N influencia a quebra de estereótipos na área?

144 respostas





# Rede Nacional de Mulheres na Nanociência

*conhecimento de inovação para cientistas e profissionais do futuro*

## OBJETIVO GERAL

Estabelecer uma **rede nacional** dedicada a **promover a inserção e participação de meninas, professoras, pesquisadoras e empreendedoras na área de Nanociências e Nanotecnologia (N&N)**

**Capacitar e a formar** uma nova geração de cientistas e profissionais, especialmente nas áreas de Ciências Exatas, Engenharias e Computação.



Esta iniciativa está ancorada e sustentada pela colaboração com centros de ensino, pesquisa e inovação de destaque acadêmico e científico nas diferentes Regiões do Brasil, visando a **distribuição equitativa e o acesso a oportunidades educacionais e de pesquisa em todas as regiões** por meio de **ações in loco** e **mentorias de pesquisadoras renomadas** na área de N&N.

### FINANCIAMENTO



# PRINCIPAIS ATIVIDADES



NANO CIRCUITOS

Portal –  
Mulheres na  
Nano

Eventos e Ações  
com Escolas

História em  
Quadrinhos

Educação  
Científica e  
Empreendedora

Produção e  
compartilhamento  
de material  
educacional

Bolsas de estudo para  
estudantes da  
educação básica (150)

Bolsas de  
estudo para  
professoras (30)

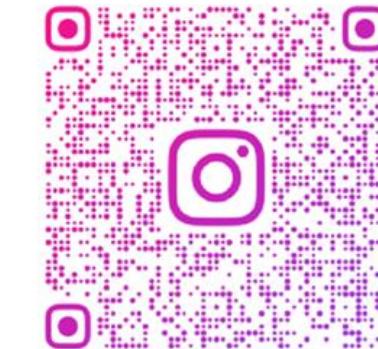
Mentorias de  
pesquisadoras

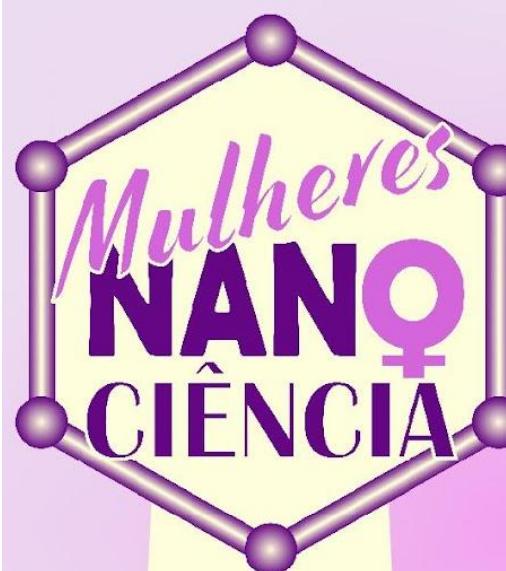
Cursos sobre Nano,  
diversidade,  
pensamento  
computacional, etc.

Apoio/CNPq: +  
1.5 milhões de  
reais



# REDE DE MULHERES NA NANOCIÊNCIA CNPq (2024-2027)





# Rede Nacional de Mulheres na Nanociência

conhecimento e inovação para cientistas e profissionais do futuro

Marcela Mohallem  
Oliveira  
UTFPR-PR.



## Comitê Gestor

Solange Binotto Fagan  
**Coordenadora do Projeto**  
UFN-RS



Alcinéia Conceição  
Oliveira  
UFC- CE



ARAUCÁRIA

CARNAÚBA

IPÊ-ROXO

MANACÁ

UMBÚ

CAMPIM DOURADO

Zélia Maria da  
Costa Ludwig  
UFJF-MG.



Rogelma Maria da  
Silva Ferreira  
UFRB-BA



Eliana Martins Lima  
UFG-GO



@REDEMULHERESNANOCIENCIAS

FINANCIAMENTO



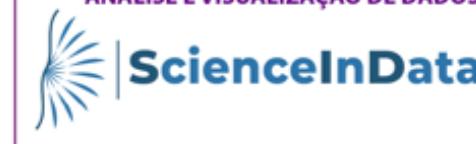
COORDENAÇÃO



COORDENAÇÃO NÚCLEOS



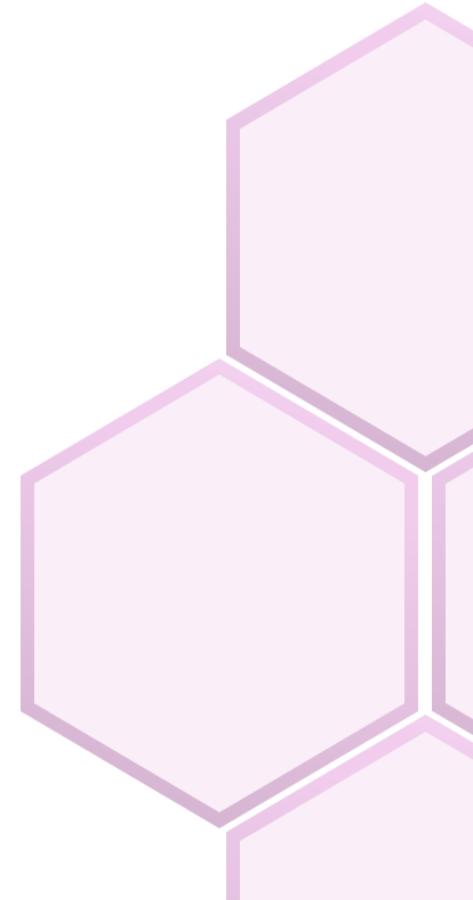
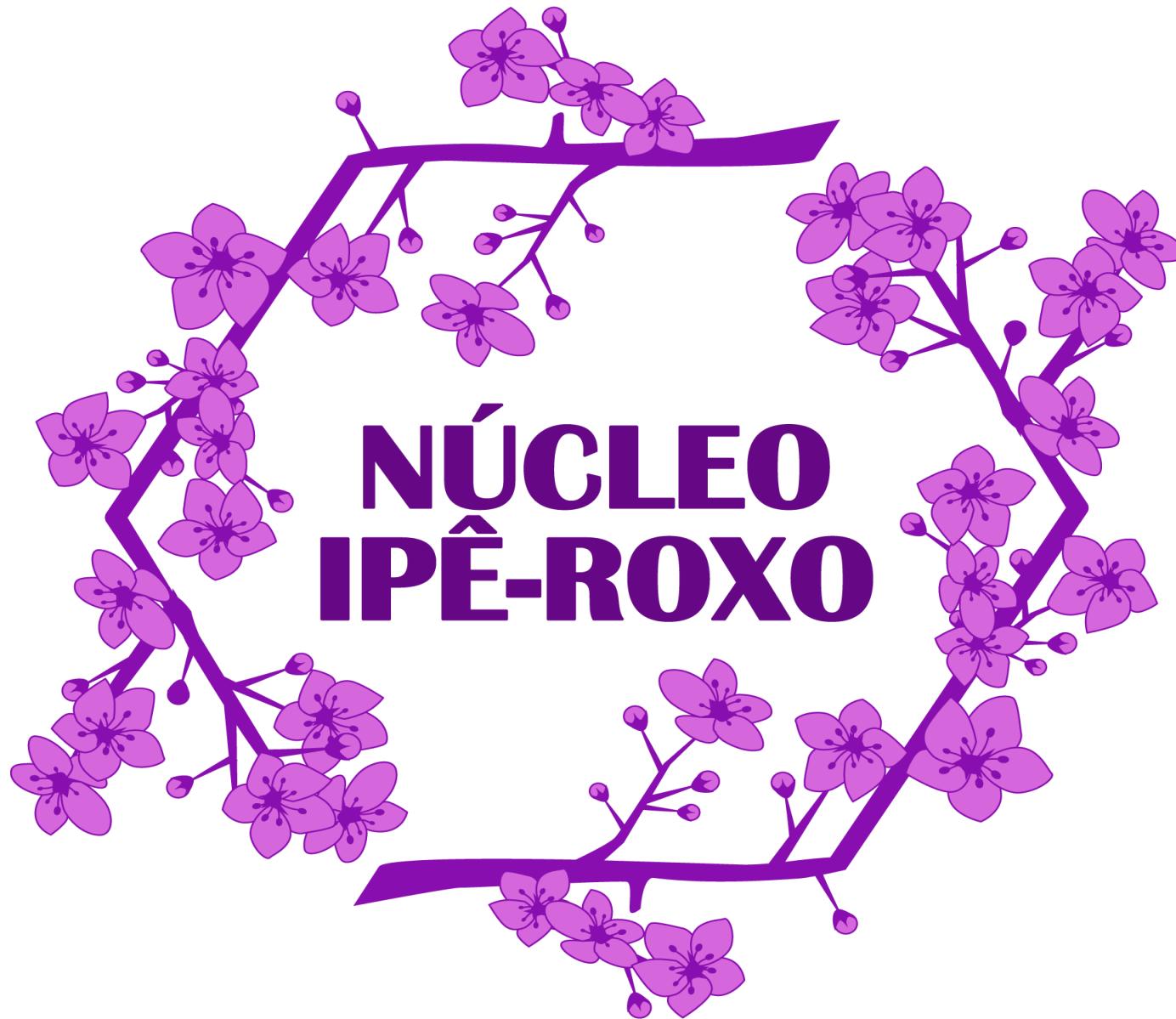
ANALISE E VISUALIZAÇÃO DE DADOS

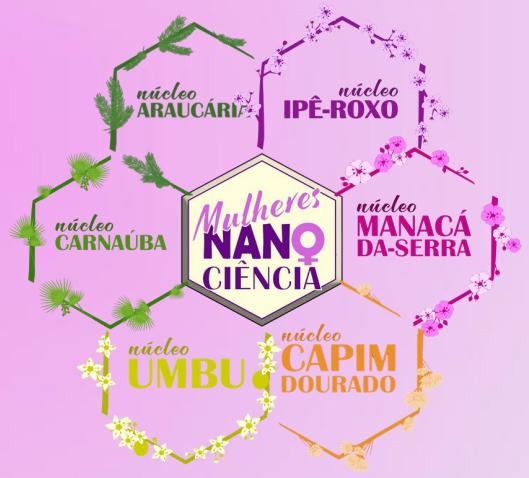


# REDE DE MULHERES NA NANOCIÊNCIA CNPq (2024-2027)



- 02 Universidades (UFN e UFRGS)
- 04 Escolas públicas e 01 privada
- 16 pesquisadoras
- 06 estudantes de pós-graduação
- 04 estudantes de graduação
- 02 bolsistas de IC - Computação (site)
- 12 bolsistas de IC Jr (Escolas)
- 02 professoras bolsistas (Escolas)
- Inúmeras voluntárias





# Jogos Educacionais



**Hello, nano-friends! Do you know about carbon nanomaterials?**

These super tiny nanomaterials, but because they are so small, they are super strong, conduct electricity and can even be invisible! Some look like very small straws, others look like thin paper or even like a ball! They're so amazing that scientists are using them to make really cool things, like glow-in-the-dark clothes and even helping doctors make people healthier!

I am NANON, made up of different carbon nanomaterials. How about want to find out more about these super tiny, super powerful materials? powerful? Let's learn by playing this trail!

**START**

The board features various hexagonal houses representing different carbon nanomaterials:

- FULLERENES-**: Made up of carbon atoms in the shape of a sphere, without dimensions (0D). Stay in this house.
- NANOTUBES-**: Made up of carbon atoms in a one-dimensional (1D) structure. Because it is a 1D material, go forward 1 space.
- DIAMOND - FULLERENE-**: Material with photovoltaic properties. You've gained energy for an extra move.
- NANOTUBES - DIAMOND-**: It is the purest and strongest form of carbon. Stay in this house for 1 round.
- NANOTUBES - DIAMOND-**: They tend to crowd together. Bring the Nanotube player to you.
- DIAMOND - FULLERENE-**: It has good biocompatibility and low toxicity. Choose 1 player to bring safely to you.
- NANOTUBES - DIAMOND-**: It is an excellent conductor of electricity. Choose a player to move 2 squares.
- NANOTUBES - FULLERENE-**: It is sturdy and can be twisted and folded without breaking. If reused, return to the beginning of the tray.
- DIAMOND - FULLERENE-**: Highly reactive. Be reactive, roll the dice again.
- GRAPHENE - DIAMOND-**: It's a transparent material. You are invisible, if you don't play for 1 round.
- GRAPHENE - DIAMOND-**: It has magnetic properties. Choose a player to pull it to you.
- NANOTUBES - DIAMOND-**: It has antioxidant and neutralizing properties. Stay in this house.
- NANOTUBES - DIAMOND-**: They have conductivity, inhibiting them from conducting and dissipating heat efficiently. Go back 2 places.

**RULES OF THE GAME:**

- 4 players
- Roll the dice and follow the order of the corresponding square

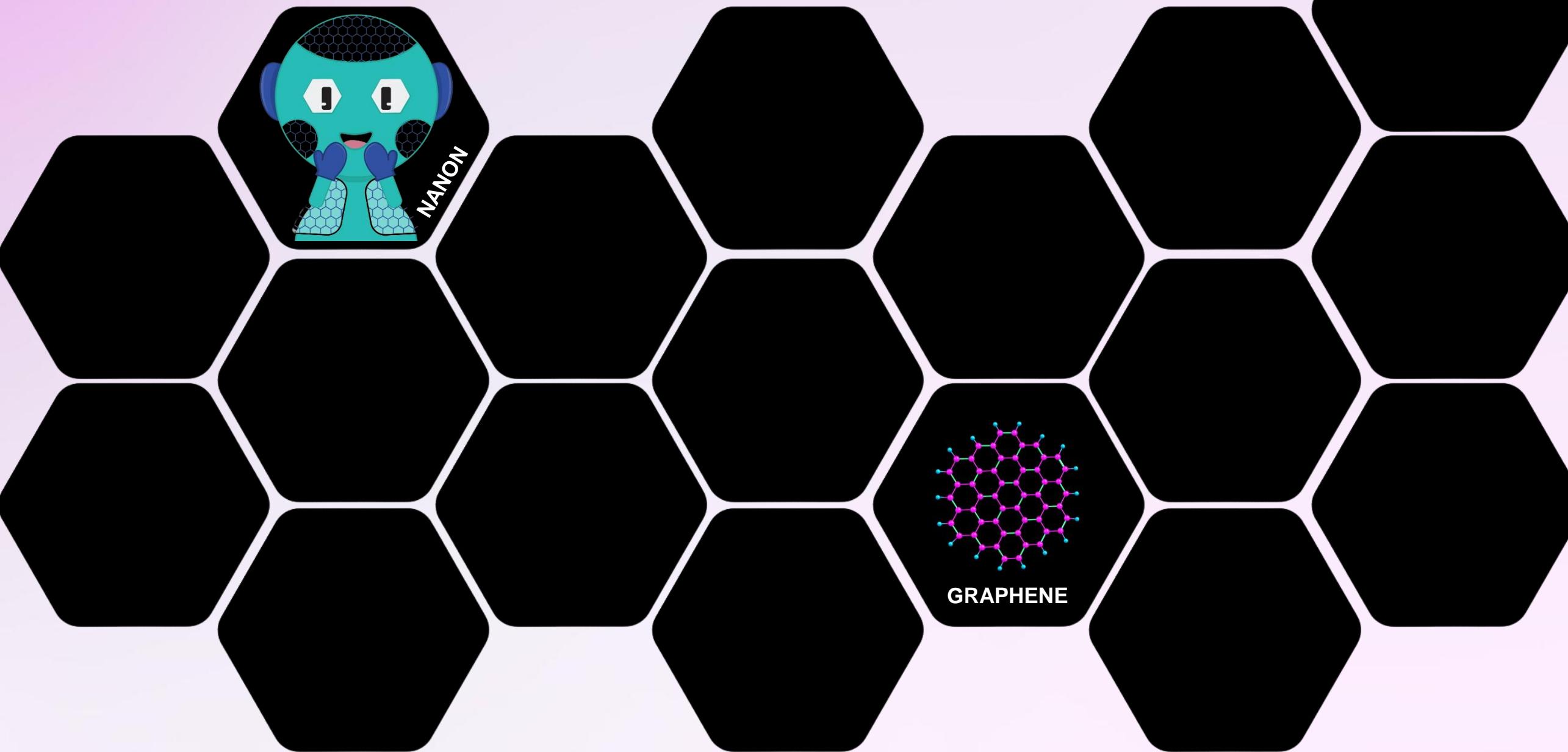
Authors: Júlia Vaz Schultz<sup>1</sup>, Ana de Souza, Anthonia Bellochio e Solange Binotto Fagan<sup>2</sup>  
ORCID ID: 1 - 0000-0002-1283-0093; 2 - 0000-0001-7878-1212

UFN Universidade Franciscana INCT Instituto Nacional de Ciência e Tecnologia em Nanomateriais de Carbono



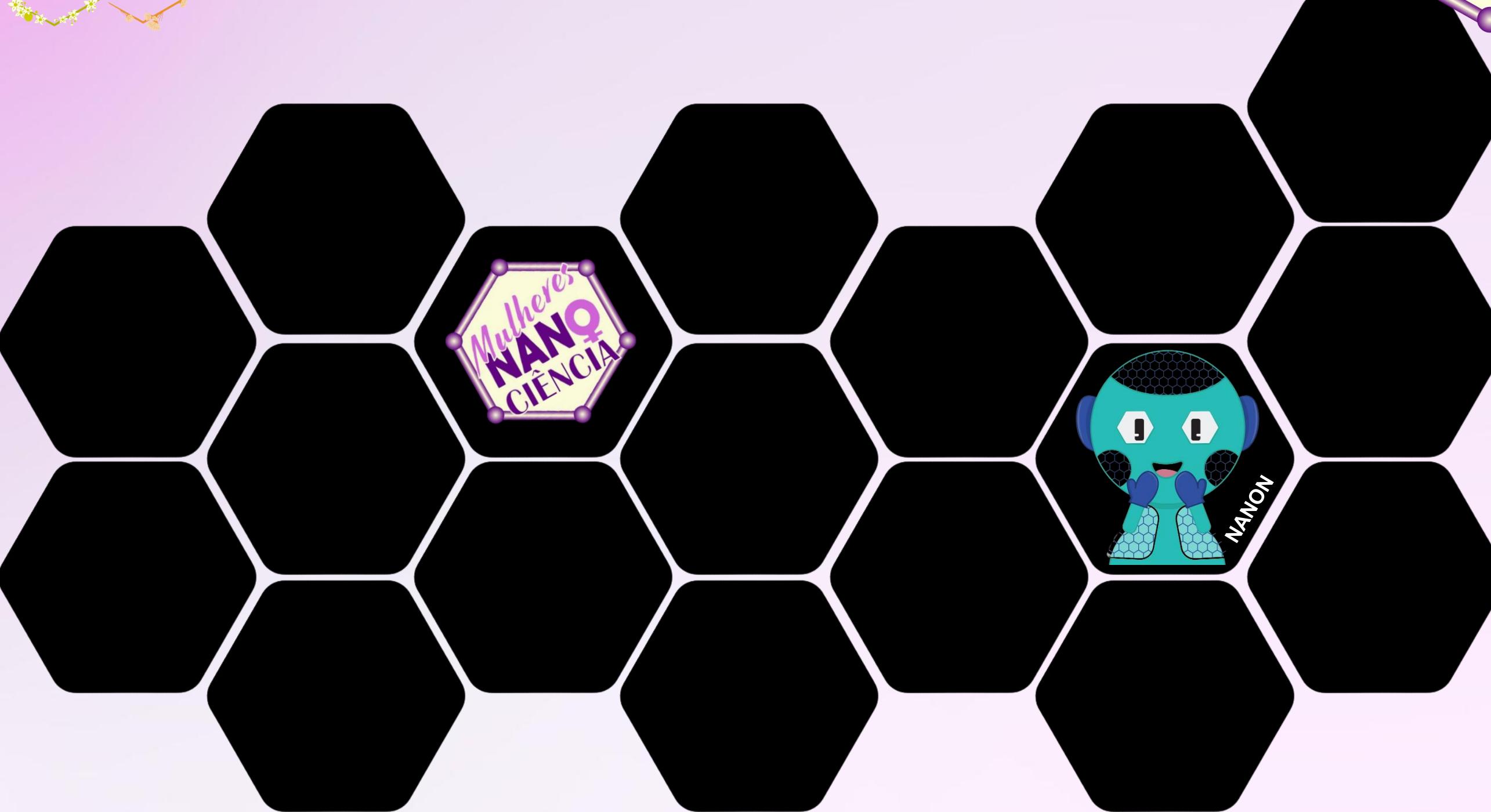


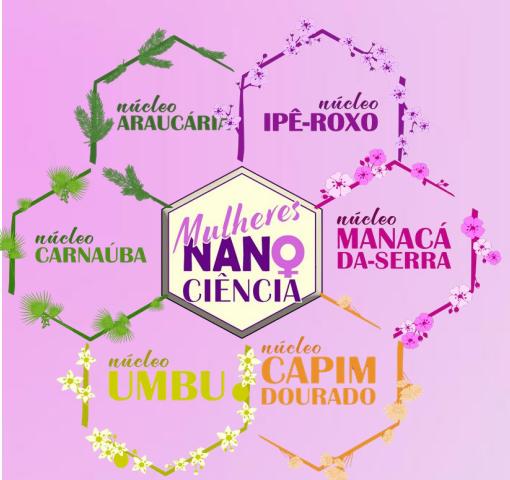
## Jogos Educacionais



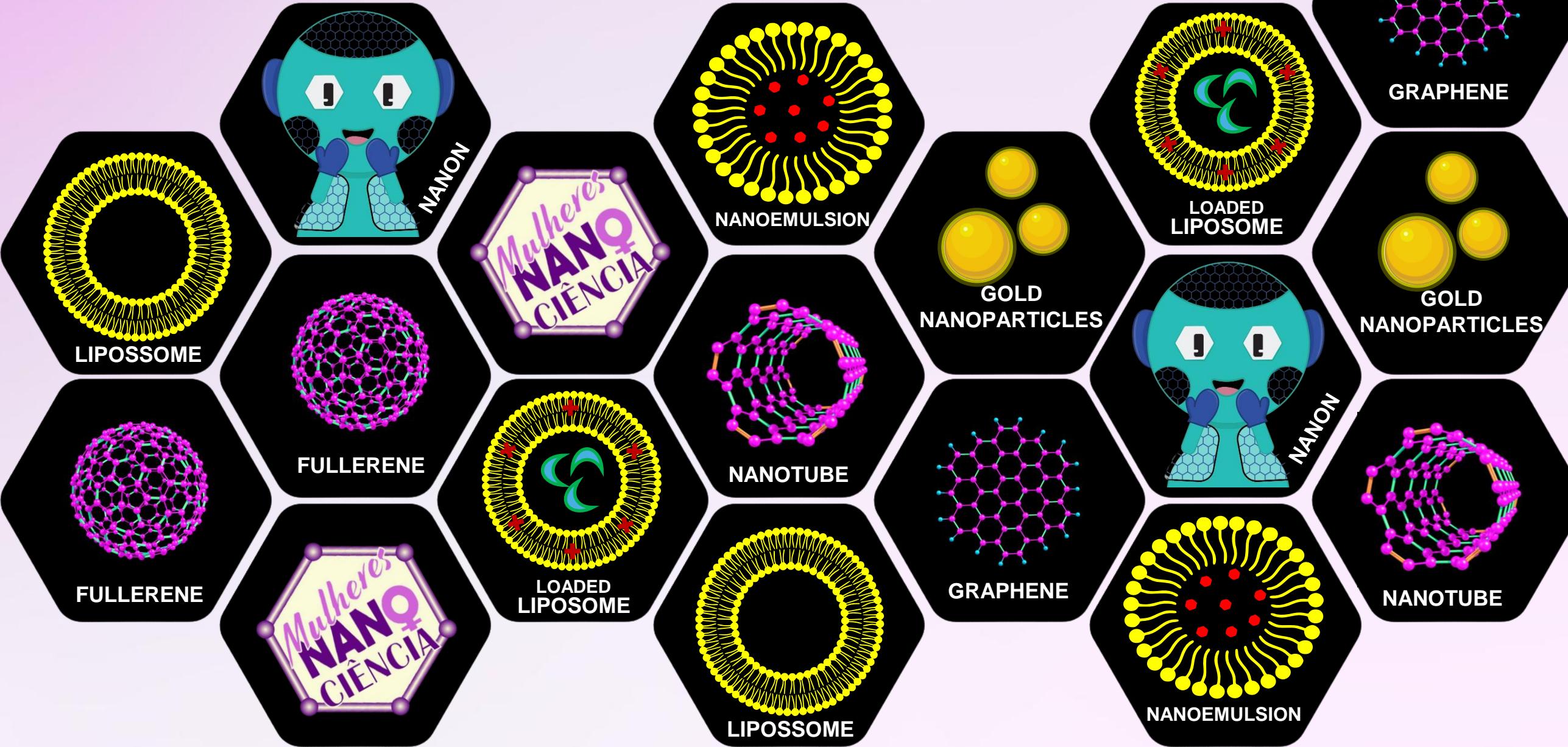


## Jogos Educacionais





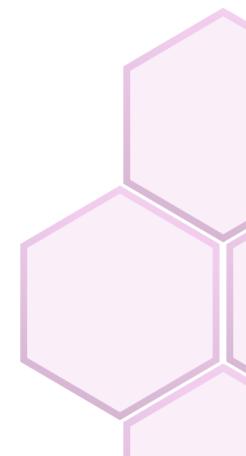
## Jogos Educacionais



## Exposições em Escolas

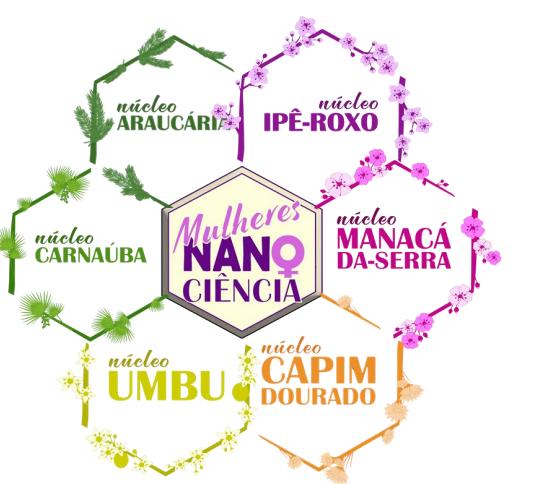


NÚCLEO  
IPÊ-ROXO

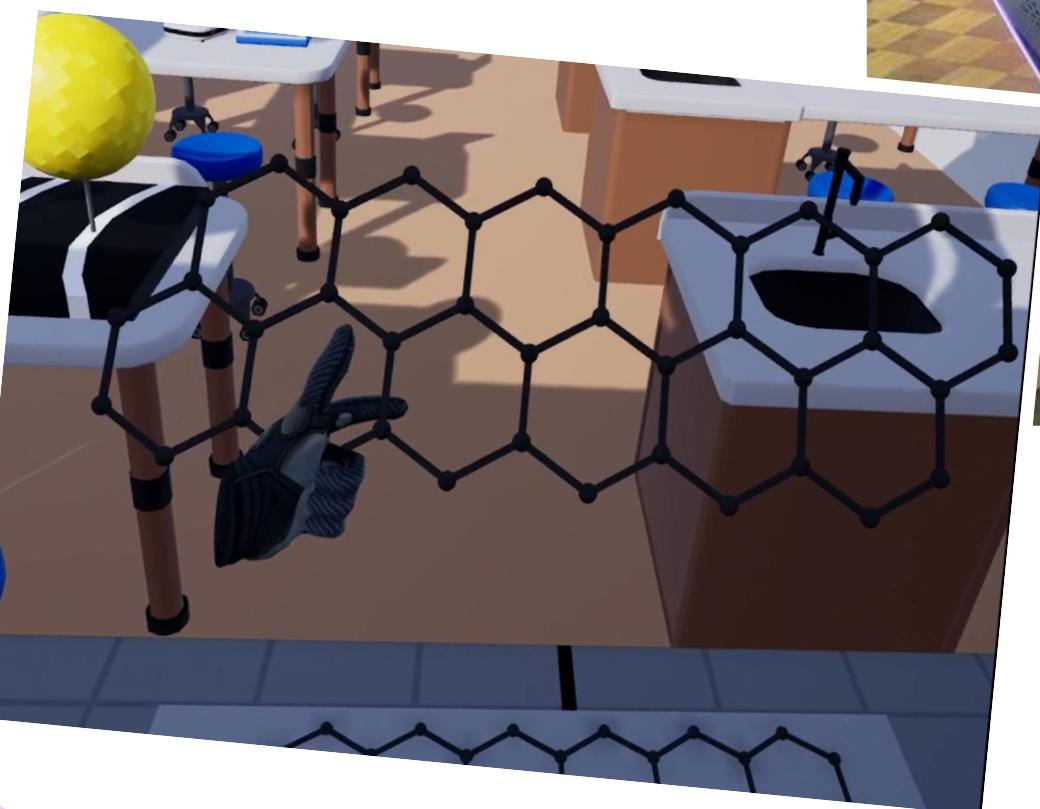
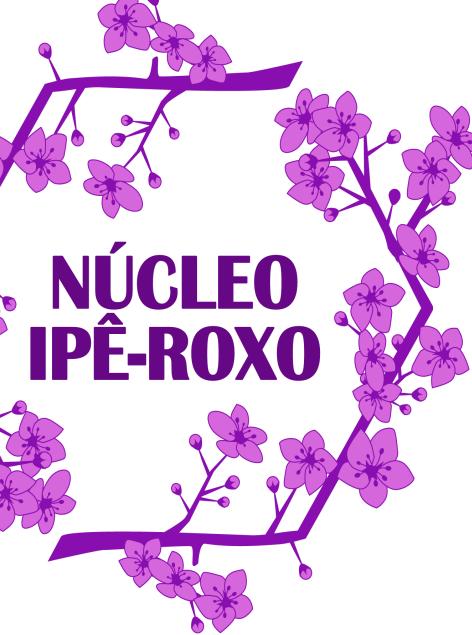
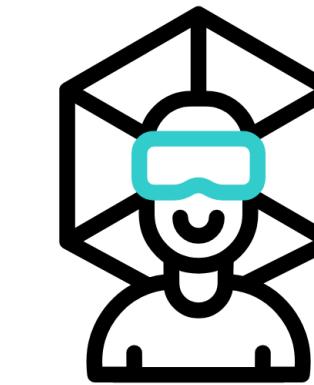
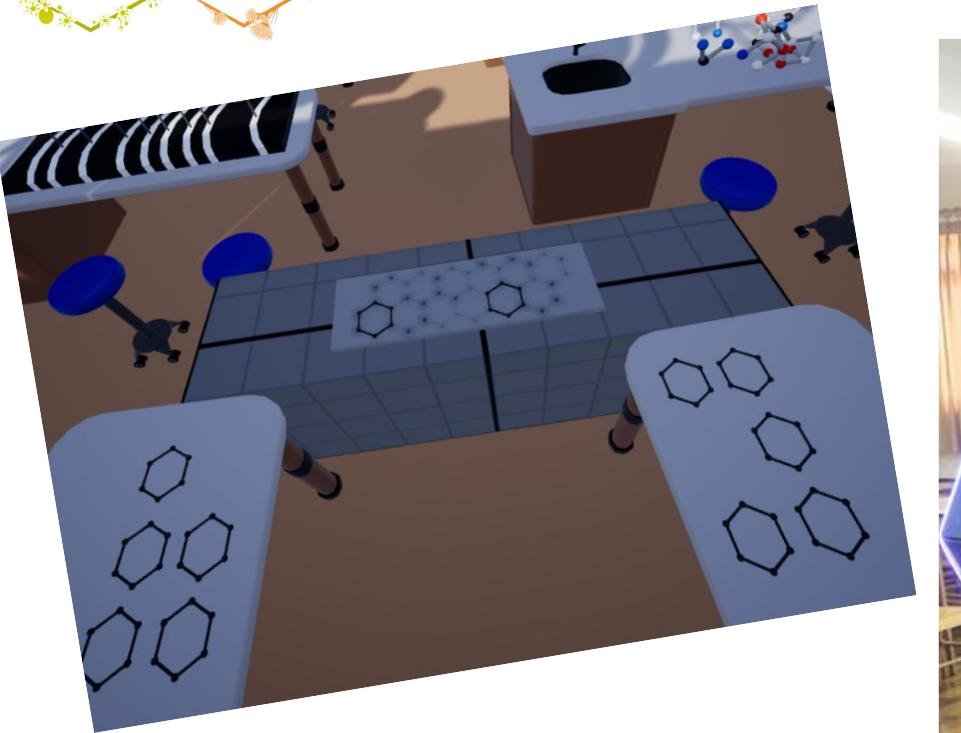


## Exposição em Escolas





## Atividades em Realidade Virtual





## Vice-reitora participa de bate-papo em Portugal sobre mulheres e meninas na ciência

Assessoria de Comunicação (ASSECOM) em 10/02/2025

Na última sexta-feira, 7 de fevereiro, a vice-reitora e professora da Universidade Franciscana (UFN), Solange Binotto Fagan, participou de um bate-papo no *International Iberian Nanotechnology Laboratory* (INL), em Braga, Portugal. O "Friday chats" ocorre semanalmente na instituição, com o objetivo de dar boas-vindas aos novos pesquisadores e promover uma discussão informal de temáticas diversas.

"A ideia foi trabalhar sobre o Dia Internacional das Mulheres e Meninas na Ciência. Fui convidada para mostrar um pouco sobre o que temos feito na UFN e (para falar) sobre a [Rede Nacional de Mulheres na Nanociência](#). Tinham muitos participantes, estava bem legal e foi significativa a participação", comenta a professora Solange.

Dentre as ações realizadas na Universidade na área de Nanociências, Solange destacou o projeto Admirável Mundo Nanométrico, a Especialização em [Ensino de Nanociências e Nanotecnologia](#), o curso EaD de Nanociências e Nanotecnologia para iniciantes, a cabine de realidade virtual, os jogos didáticos, as oficinas em escolas, e a publicação do livro "[Admirável Mundo Nanométrico](#)".

A professora também comentou sobre a Rede Nacional de Mulheres na Nanociência. O projeto envolve 21 Instituições de Ensino Superior (IES), quatro empresas e 20 escolas de Educação Básica. O principal objetivo da Rede é **capacitar e formar uma nova geração de cientistas e profissionais**, gerando distribuição equitativa e o acesso a oportunidades educacionais e de pesquisa em todas as regiões do Brasil.



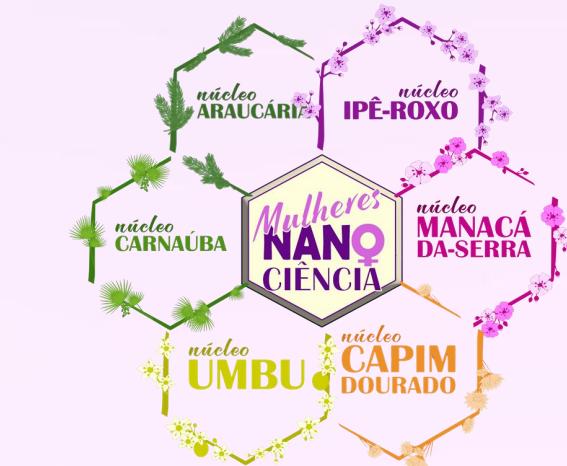
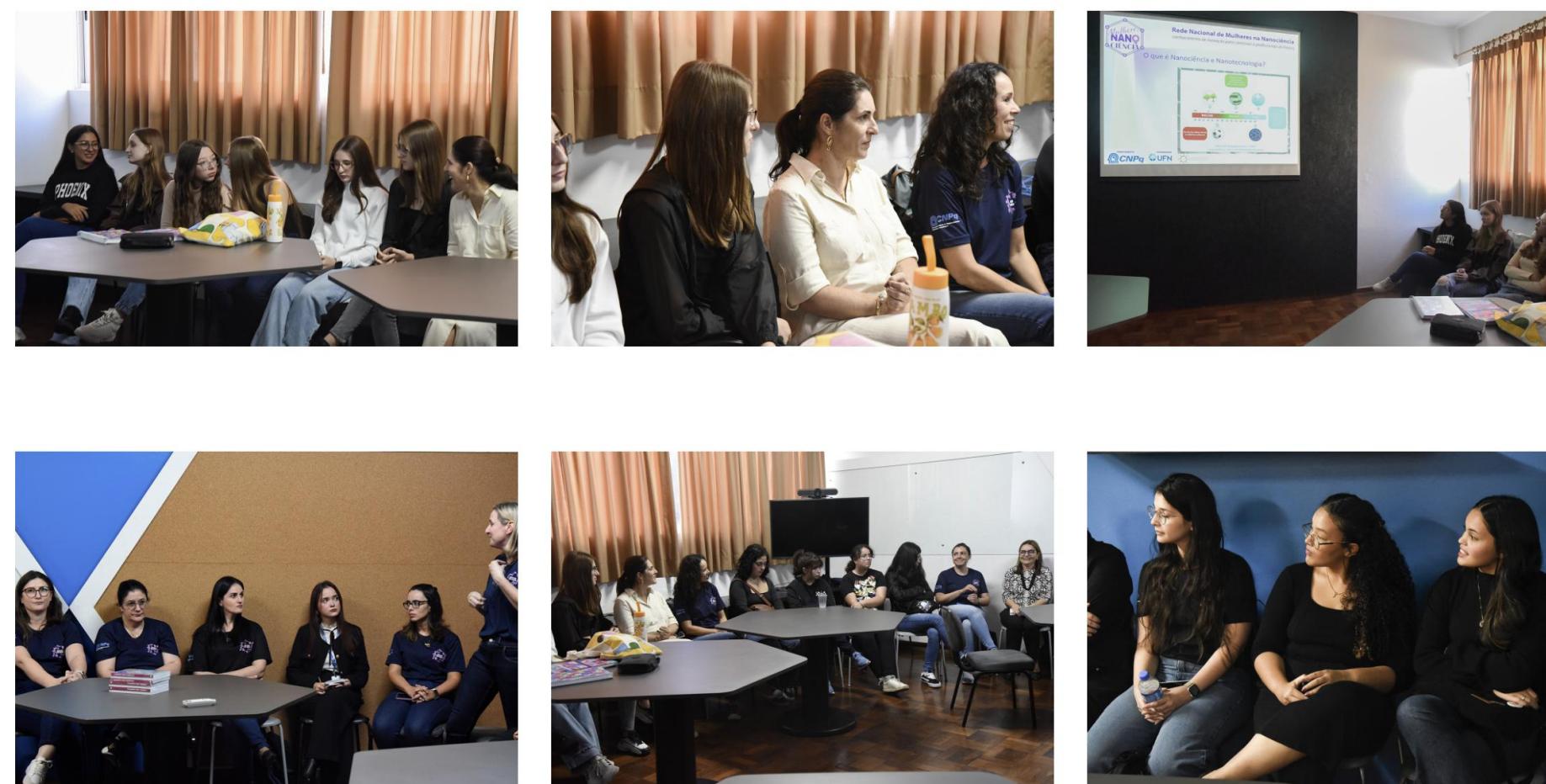


# Primeiro encontro da Rede Nacional de Mulheres na Nanociência é realizado na UFN

Assessoria de Comunicação (ASSECOM) em 24/04/2025

A Universidade Franciscana (UFN), deu início a um projeto inovador voltado para a inclusão e empoderamento de mulheres e meninas nas áreas de Nanociência e Nanotecnologia. A primeira reunião da **Rede Nacional de Mulheres na Nanociência** foi realizada na quarta-feira (23) e reuniu estudantes, pesquisadoras e educadoras com o objetivo de incentivar a participação feminina em áreas de Ciência, Tecnologia e Inovação.

Durante o encontro a vice-reitora da UFN e coordenadora do projeto, professora Solange Binotto Fagan, destacou a importância do acompanhamento das participantes. "O que nós temos como coordenadores do projeto é que vamos conduzir as participantes por no mínimo cinco anos. Vamos estar de alguma forma com vocês depois do projeto, tanto se decidirem ir para área, se foram fazer uma faculdade, se forem para uma área acadêmica ou se tornaram empresárias. A ideia é





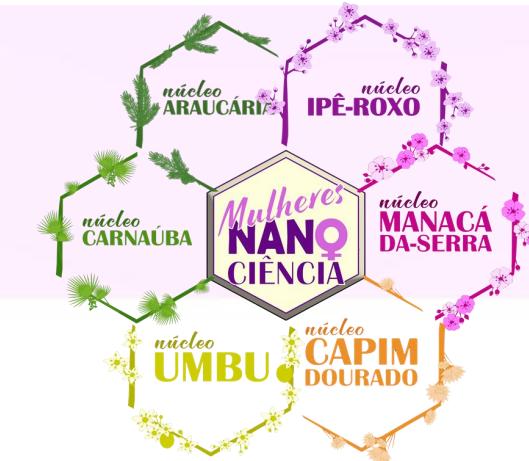
# Rede Nacional de Mulheres na Nanociênci

conhecimento de inovação para cientistas e profissionais do futuro



**NANOCIRCUITO: DO ÁTOMO  
AO DISPOSITIVO: SIMULAÇÃO  
COMPUTACIONAL**

14/05/25



**Mulheres  
NANO  
CIÊNCIA**

**Rede Nacional de Mulheres na Nanociência**  
*conhecimento de inovação para cientistas e profissionais do futuro*

**Impressão 3D**  
**25/06/25**

A photograph showing a group of students in a workshop setting. In the background, there is a large screen displaying the text "NANOCIRCUITO" and "Como transformar ideias em realidade com impressão 3D". To the left, there is a banner for "PROEXX-PG" and a small rocket-shaped display.

## Rede de Mulheres na Nanociência promove oficina de impressão 3D para estudantes

Assessoria de Comunicação (ASSECOM) em 26/06/2025

Na última quarta-feira, 25 de junho, foi realizada uma etapa do **Nanocircuito** da [Rede Nacional de Mulheres na Nanociência](#). Alunas de escolas vinculadas à iniciativa acompanharam a atividade na **Cidade da Ciência**, no [ITEC Park](#), da Universidade Franciscana (UFN). As estudantes tiveram a oportunidade de participar da oficina "**Como transformar ideias em realidade com impressão 3D**". O objetivo era incentivar o uso de novas tecnologias no desenvolvimento de **soluções inovadoras**.

"A ideia foi trabalhar a questão da impressão 3D e da prototipagem para, a partir desse Nanocircuito, elas começarem a pensar nos seus **produtos**. Foi muito interessante porque muitas delas ficaram extremamente encantadas, inclusive, as professoras das escolas que estavam acompanhando, para poder realizar esse tipo de atividade e, quem sabe, adquirir também as impressoras nas escolas", afirma a coordenadora da [Rede](#) e Vice-reitora da UFN, professora **Solange Binotto Fagan**.

O Nanocircuito reuniu professoras, bolsistas e voluntárias da Rede. "Usamos a impressão 3D para divulgar a ciência, especialmente, no desenvolvimento de **jogos educativos** e **materiais auxiliares para o ensino de Nanociências**. O nosso propósito com o Nanocircuito foi apresentar e desmistificar a tecnologia, incentivar a criatividade, compartilhar nossas experiências com a manufatura aditiva e instigar o pensamento criativo atrelado à pesquisa científica e ao desenvolvimento tecnológico", explica a doutoranda do [Programa de Pós-graduação em Nanociências](#), **Júlia Vaz Schultz**.

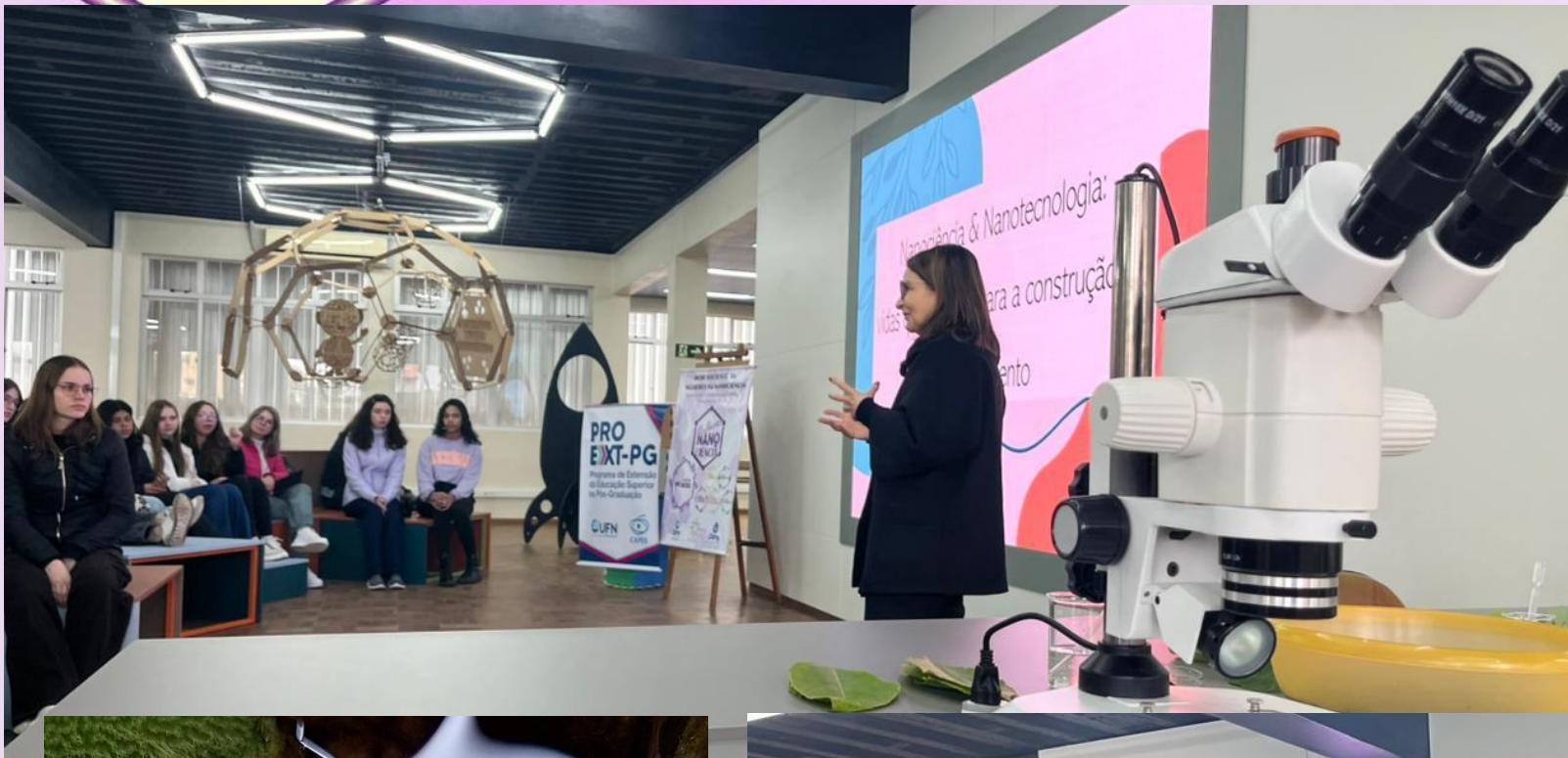
As alunas que participaram da oficina são da Escola Estadual de Ensino Médio Cilon Rosa, da Escola de Ensino Fundamental Irmão Quintino, do Colégio Franciscano Sant'Anna, da Escola Estadual de Ensino Fundamental Padre Rafael Iop, e do Instituto Estadual de Educação Olavo Bilac.





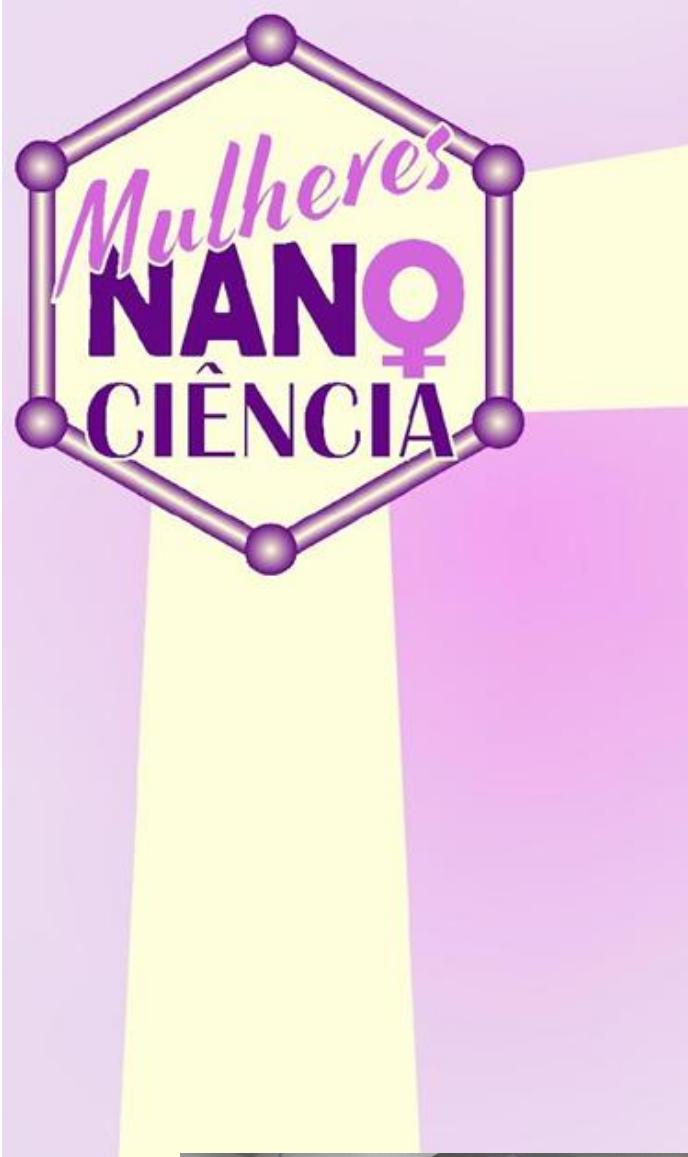
# Rede Nacional de Mulheres na Nanociência

*conhecimento de inovação para cientistas e profissionais do futuro*



**Nanociência e  
Nanotecnologia: vidas que  
inspiram o conhecimento  
23/07/25**





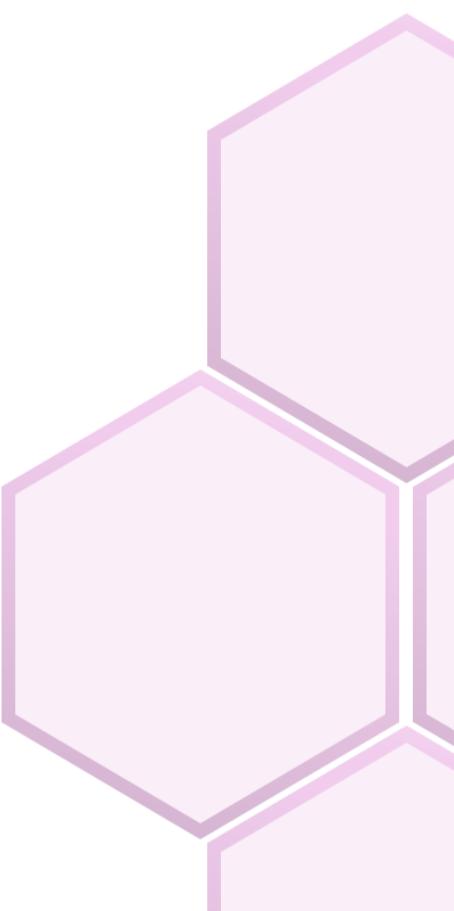
# Rede Nacional de Mulheres na Nanociênciа

conhecimento de inovação para cientistas e profissionais do futuro



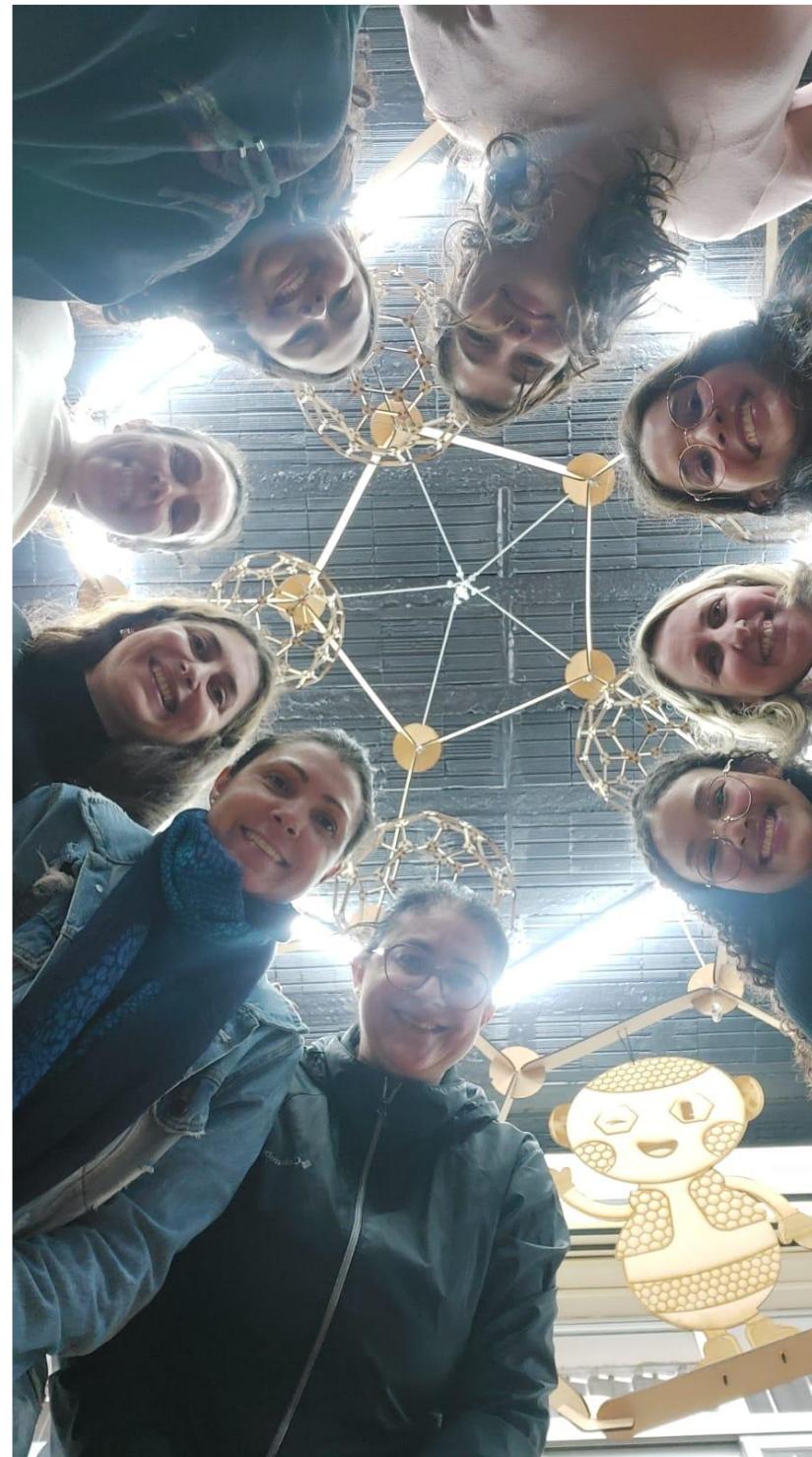
FINANCIAMENTO





# Espaços Educativos

## Cidade da Ciência - UFN



# PORTAL – REDE MULHERES NA NANOCIÊNCIA

[redemulheresnanociencias@gmail.com](mailto:redemulheresnanociencias@gmail.com) [redemulheresnanociencias](https://www.instagram.com/redemulheresnanociencias) [youtube.com/@redemulheresnano](https://youtube.com/@redemulheresnano)

REDE NACIONAL DE MULHERES NA NANOCIÊNCIA

PROJETO ▾

EQUIPE ▾

INSTITUIÇÕES E EMPRESAS ▾

PRODUTOS EDUCACIONAIS

GALERIA ▾

CONTATO

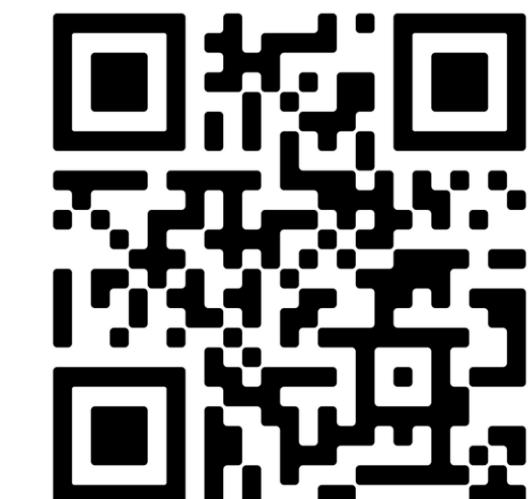
LOGIN

# REDE NACIONAL DE MULHERES NA NANOCIÊNCIA

Conhecimento e Inovação para Cientistas e Profissionais do  
Futuro

[SAIBA MAIS](#)

[CONTATO](#)



# INSTAGRAM – REDE MULHERES NA NANOCIÊNCIA

Últimos 30 dias

2 de mai - 31 de mai

22,512 Visualizações

58,9% Seguidores • 41,1% Não seguidores

Contas alcançadas 6,325 +317,8%

Gênero

28,1% Homens • 71,9% Mulheres

Público

Principais cidades

Cidade	Porcentagem
Santa Maria (Rio Grande do Sul)	37,6%
Juiz de Fora	7,9%
Aracaju	4,6%
Belo Horizonte	3,4%

Principais faixas etárias

Faixa Etária	Porcentagem
25-34	30,1%
35-44	25,9%
45-54	17,5%
18-24	16,9%

Principais países

País	Porcentagem
Brasil	97,9%
Portugal	0,8%
Peru	0,2%
Argentina	0,2%

@REDEMULHERESNANOCIENCIAS

# YOUTUBE – REDE MULHERES NA NANOCIÊNCIA

## @redemulheresnano

The screenshot shows the YouTube channel interface for 'Rede Nacional de Mulheres na Nanociências'. On the left, the YouTube sidebar includes links for Podcasts, Mais do YouTube (YouTube Premium, Studio, Music, Kids), Configurações, Histórico de denú..., Ajuda, and Enviar feedback. Below the sidebar is a large QR code.

The main content area features the channel's logo, 'Mulheres NANO CIÊNCIA', and a video thumbnail titled 'ARAUCÁRIA IPÉ-ROXO'. The video has 1:14:44 duration and 82 subscribers. The channel description reads: 'Estabelecer uma rede nacional dedicada a promover a participação e o desenvolvimento ...mais' and provides a link to Instagram: [instagram.com/redemulheresnanociencias?igsh=MXUwdndlejBseXdyA==](https://instagram.com/redemulheresnanociencias?igsh=MXUwdndlejBseXdyA==).

Below the video thumbnail is a grid of logos for six nanoscience hubs: 'núcleo CAMPIM DOURADO' (orange), 'núcleo UMBU' (yellow), 'núcleo MANACÁ DA-SERRA' (pink), 'núcleo IPÉ-ROXO' (purple), 'núcleo ARAUCÁRIA' (green), and 'núcleo CARNAÚBA' (light green). To the right of the video thumbnail is a purple banner with the text 'REDE NACIONAL DE MULHERES NA NANOCIÊNCIA O CONHECIMENTO E A INOVAÇÃO PARA CIENTISTAS E PROFISSIONAIS DO FUTURO'.

On the right side of the screen, there is a promotional graphic for a webinar. The title is 'Webinar: CÂNCER DE MAMA E PRESERVAÇÃO DA FERTILIDADE'. It features a portrait of the speaker, 'Rodrigo Maurer', and includes details about the event: 'Palestrante: Rodrigo Maurer', 'Data: 08 de Maio de 2025', 'Horário: 16:00 horas', and 'Local: Canal do YouTube @redemulheresnano'. Logos for CNPq and UFSC are visible at the bottom of the graphic.



# AUTUMN MEETING 2026

## BRAZILIAN PHYSICAL SOCIETY

**May 17 - 21**  
**Cuiabá, MT - Brazil**

**Teldo Anderson da Silva Pereira – UFMT**

Coordenador Geral

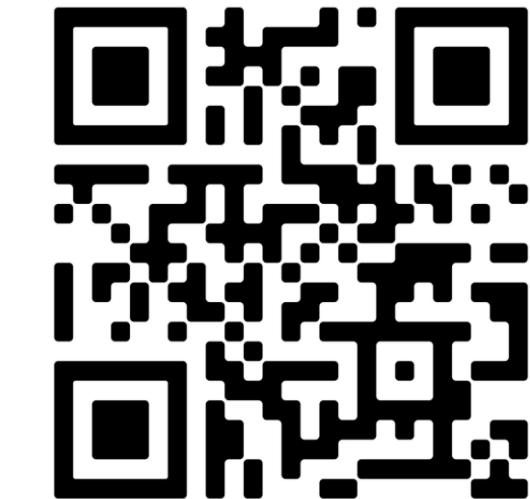
**Solange Binotto Fagan – UFN**

Coordenadora de Programa

<https://www1.fisica.org.br/~eosbf/2026/index.php/en/>



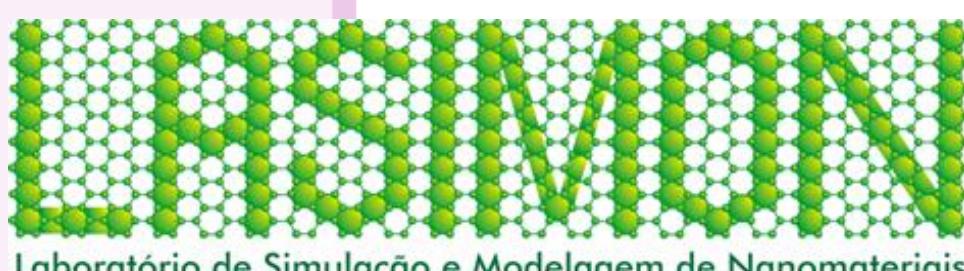
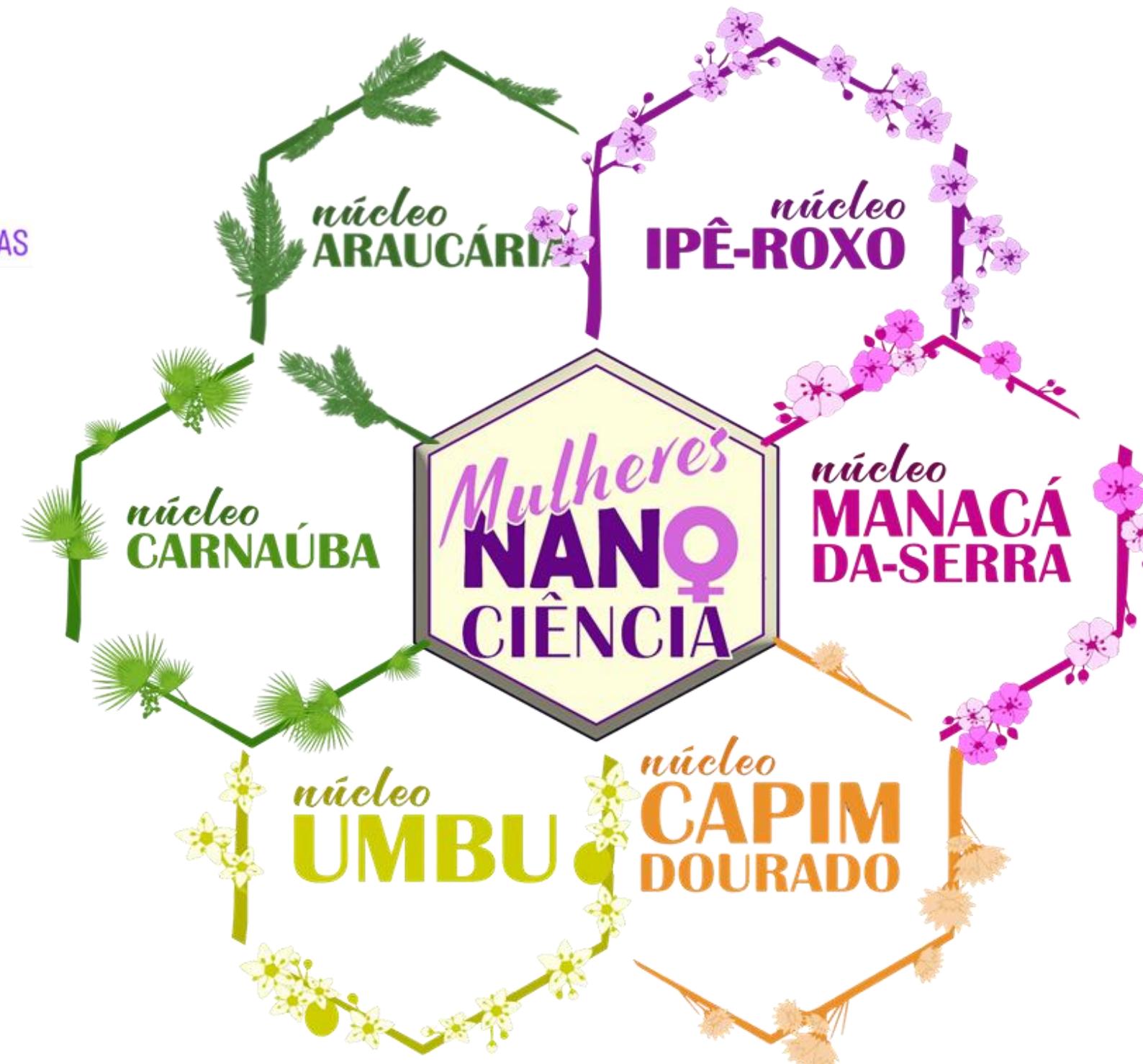
SITE



YOUTUBE



# Obrigada!



Laboratório de Simulação e Modelagem de Nanomateriais



@SOLANGEBINOTTOFAGAN



@REDEMULHERESNANOCIENCIAS