

1 2 9 0



UNIVERSIDADE D
COIMBRA



Café com Física
12/06/2025

Simulational contributions to address water emerging contaminant pollution

JOSÉ RAFAEL BORDIN

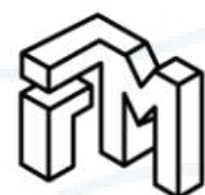
DEPARTAMENTO DE FÍSICA

PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA

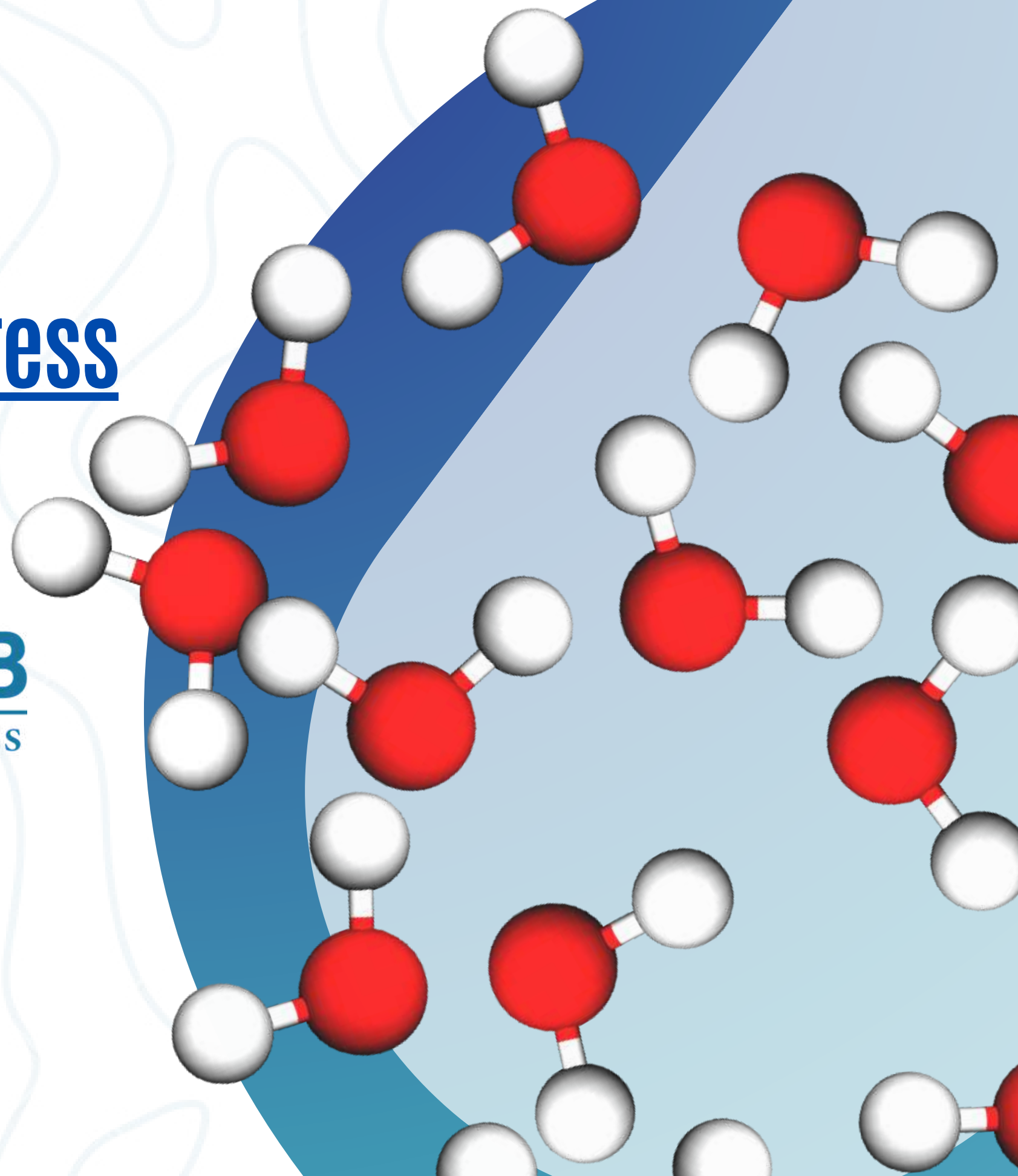
UNIVERSIDADE FEDERAL DE PELOTAS



BORDIN LAB
SOFT MATTER PHYSICS



INSTITUTO DE
FÍSICA E
MATEMÁTICA





- **WHERE AND WHO WE ARE**
- **WATER IS STRANGE**
- **WHY WE SHOULD BE REALLY CONCERNED WITH CONTAMINANTS OF EMERGING CONCERN**
- **DEVELOPING NANOMATERIALS WITH REALLY LOW BUDGET AND NO LAB**
- **SOME SIMULATIONAL RESULTS**
- **TAKE HOME MESSAGES**



Pelotas



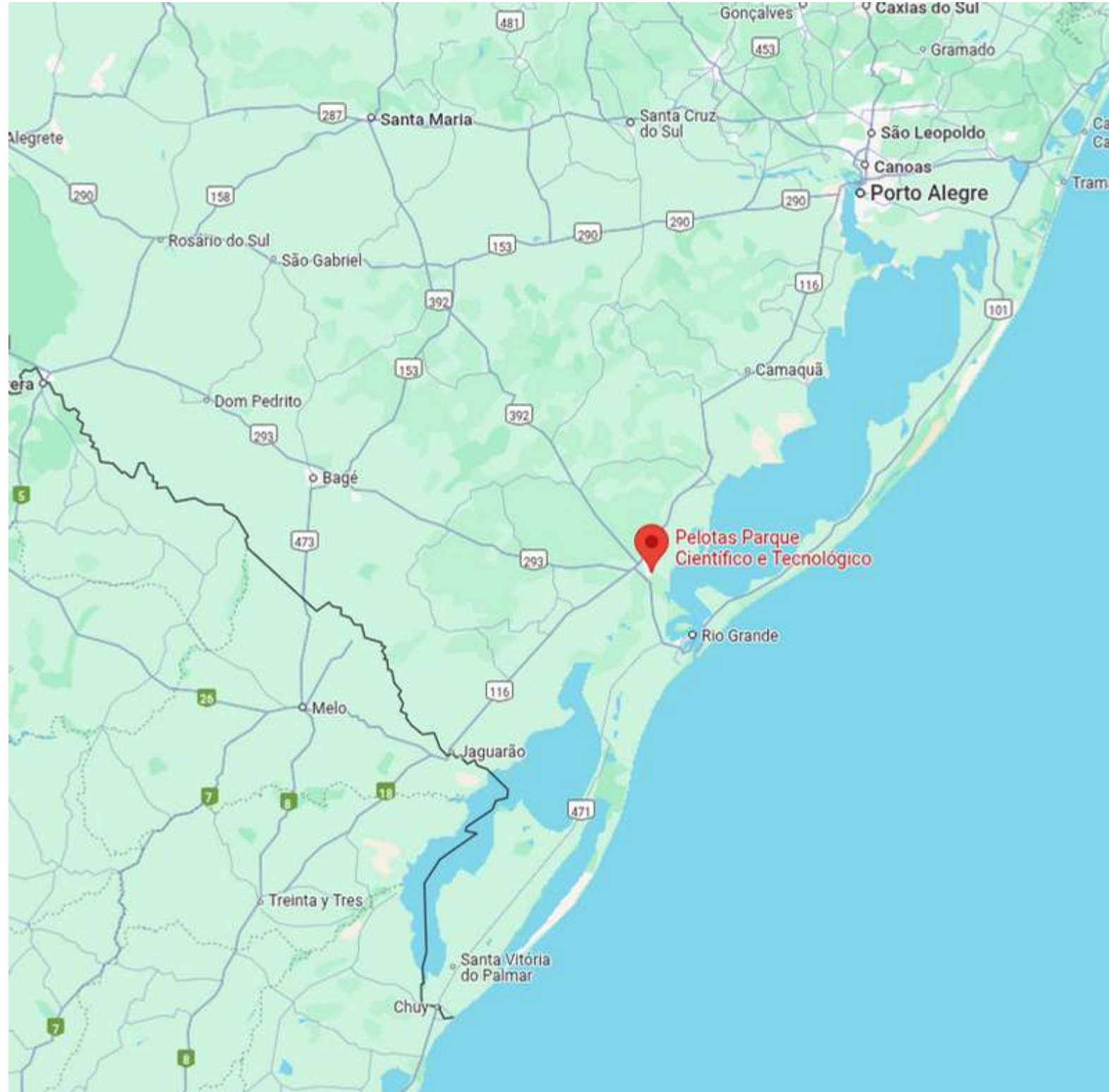
WATER AT NANOSCALE



Pelotas



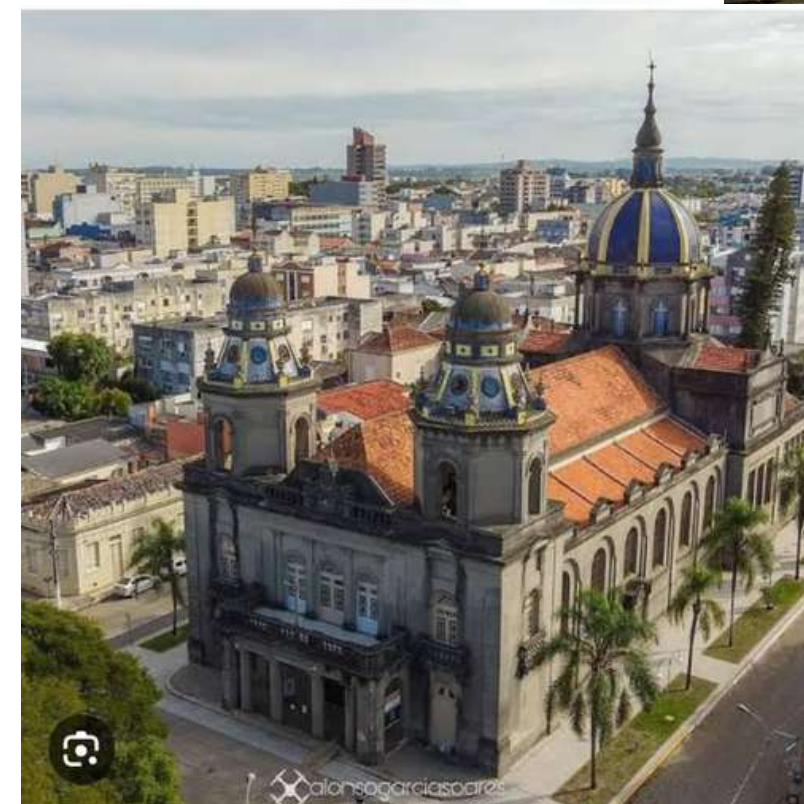
WATER AT NANOSCALE



RAFA MARIN
fotografia



Pelotas



WATER AT NANOSCALE

Pelotas



gov.br

Órgãos do Governo Acesso à Informação Legislação Acessibilidade Entrar com o gov.br

Ministério do Turismo

O que você procura?



Assuntos > Notícias > Pelotas (RS) é oficialmente a Capital Nacional do Doce; título deve contribuir para impulsionar o turismo local

TÍTULO NACIONAL

Pelotas (RS) é oficialmente a Capital Nacional do Doce; título deve contribuir para impulsionar o turismo local

A concessão do título ganha ainda mais relevância num momento de tanta dificuldade pela qual passam 90% dos municípios gaúchos

Publicado em 03/06/2024 15h04

Compartilhe: f x in @



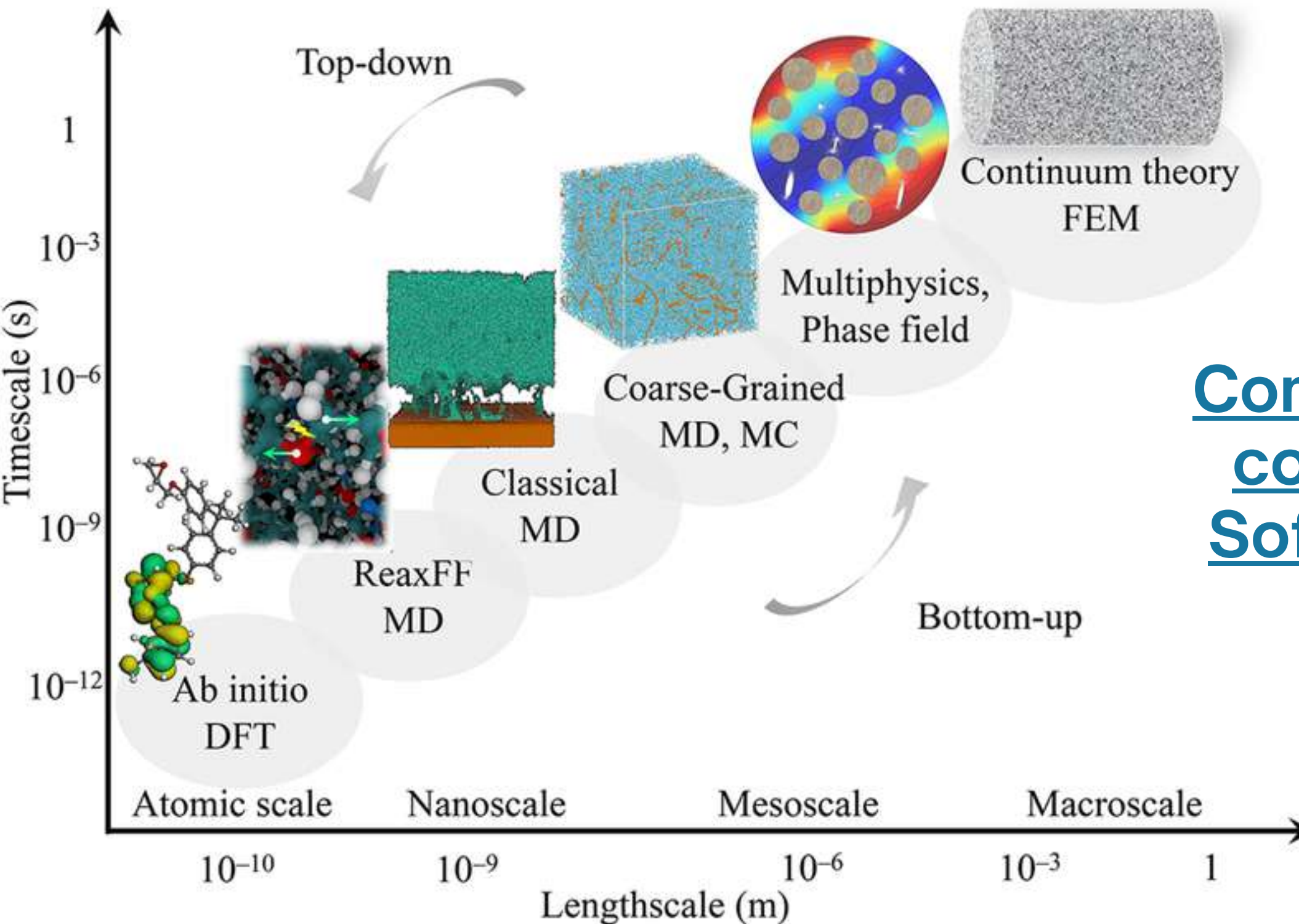
WATER AT NANOSCALE

UFPEl



WATER AT NANOSCALE

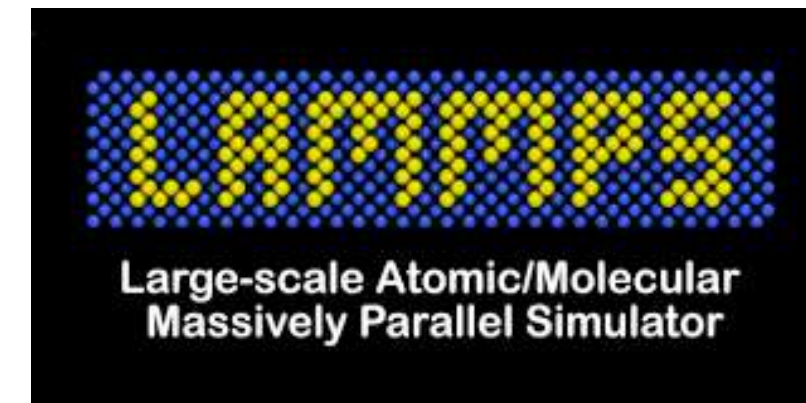




Computational modeling of collective phenomena in Soft and Biological Matter

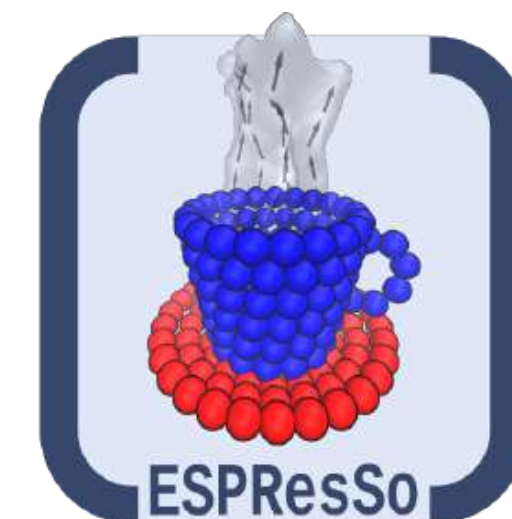


Packages:

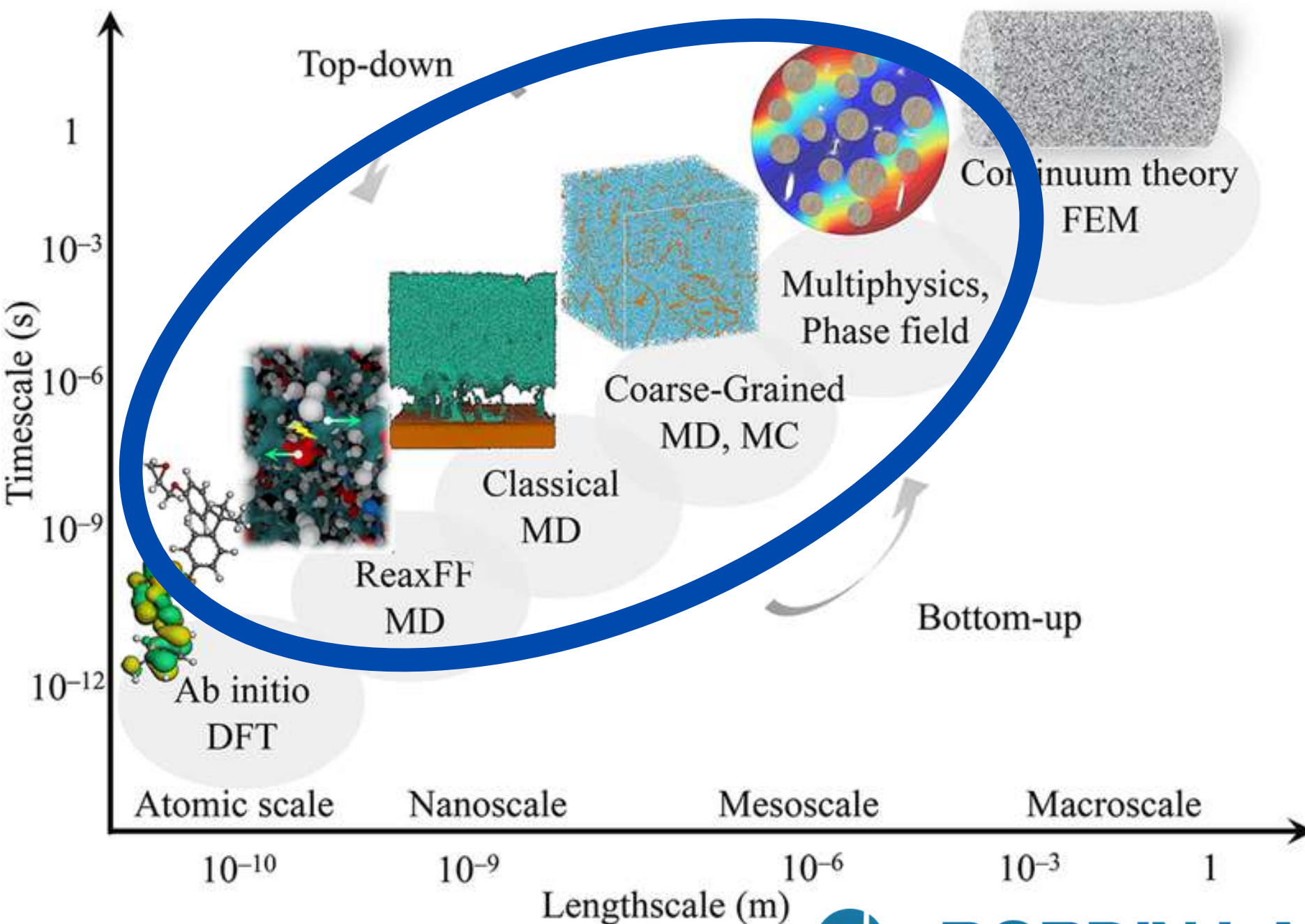


Gromacs

fast
flexible
free



Home made codes



BORDIN LAB
SOFT MATTER PHYSICS



SOCIOPHYSICS

FLUIDS



COLLOIDS



NANOMATERIALS



BIO/MEDICAL PHYSICS



water



is strange

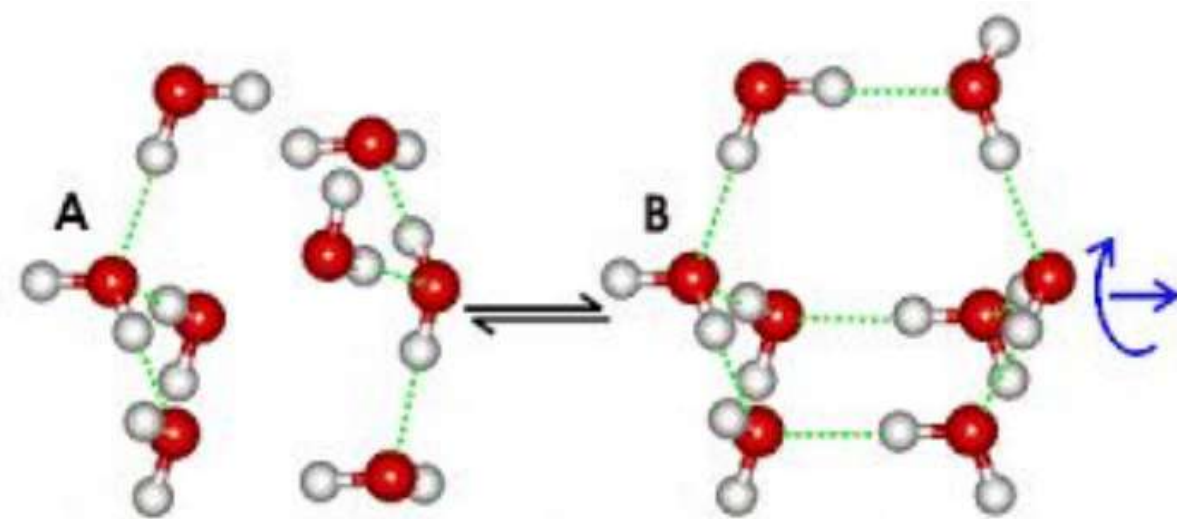
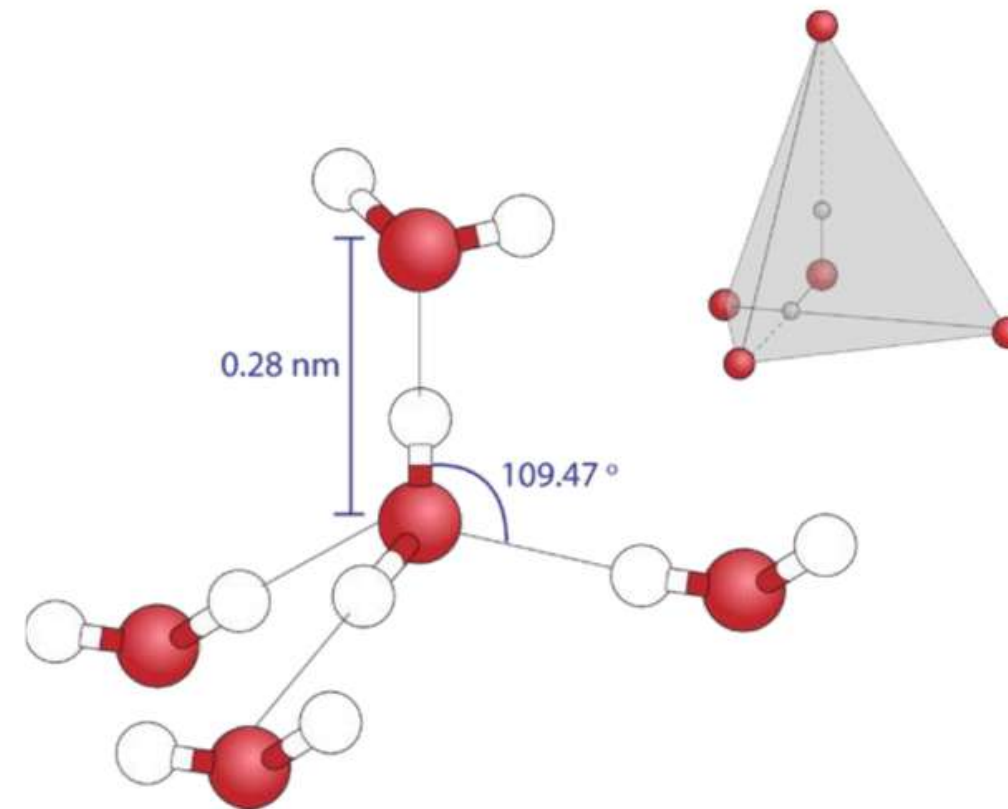
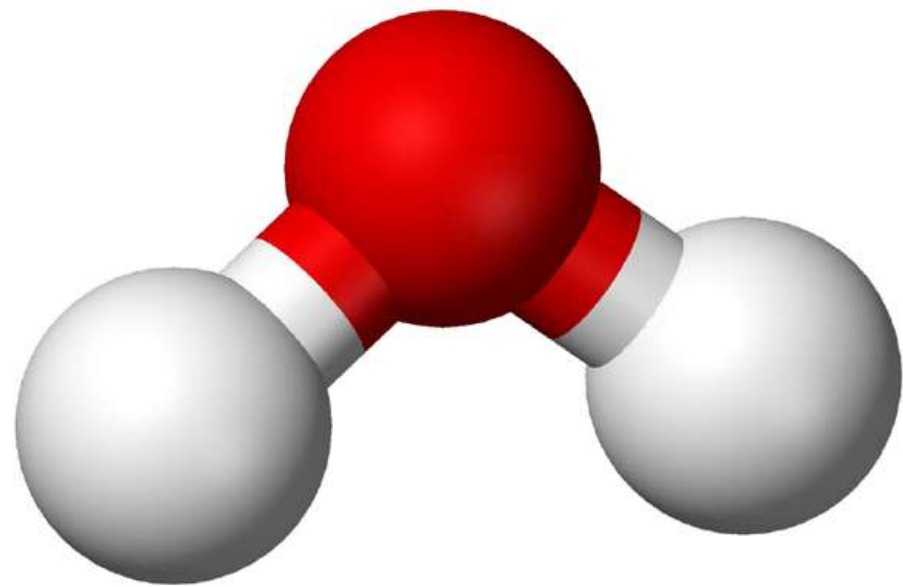


WATER AT NANOSCALE



water

simple, yet not trivial



simple molecule made with two of the most common elements in the Universe

> 70 known anomalies

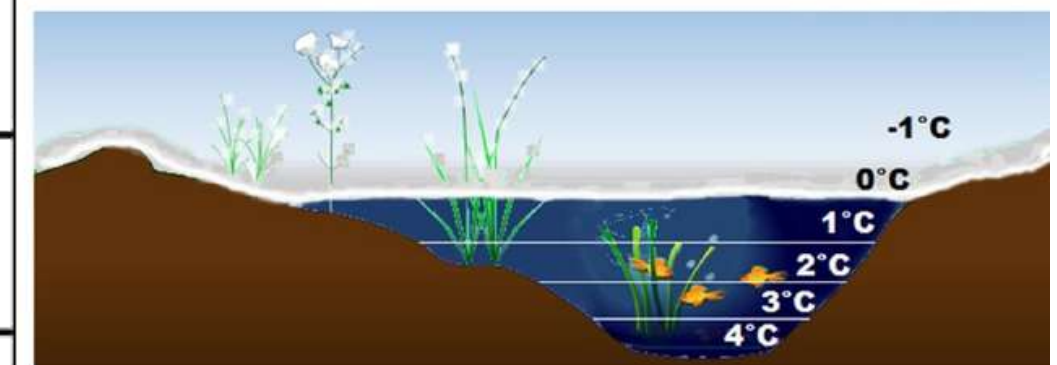
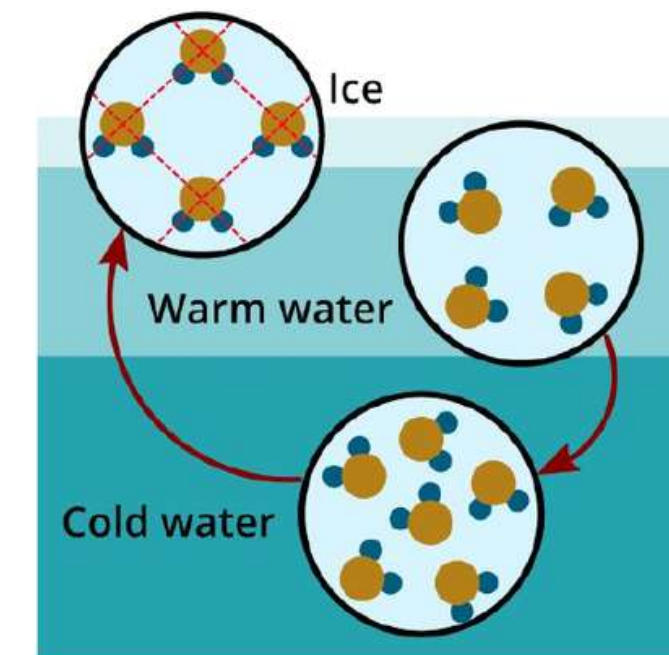
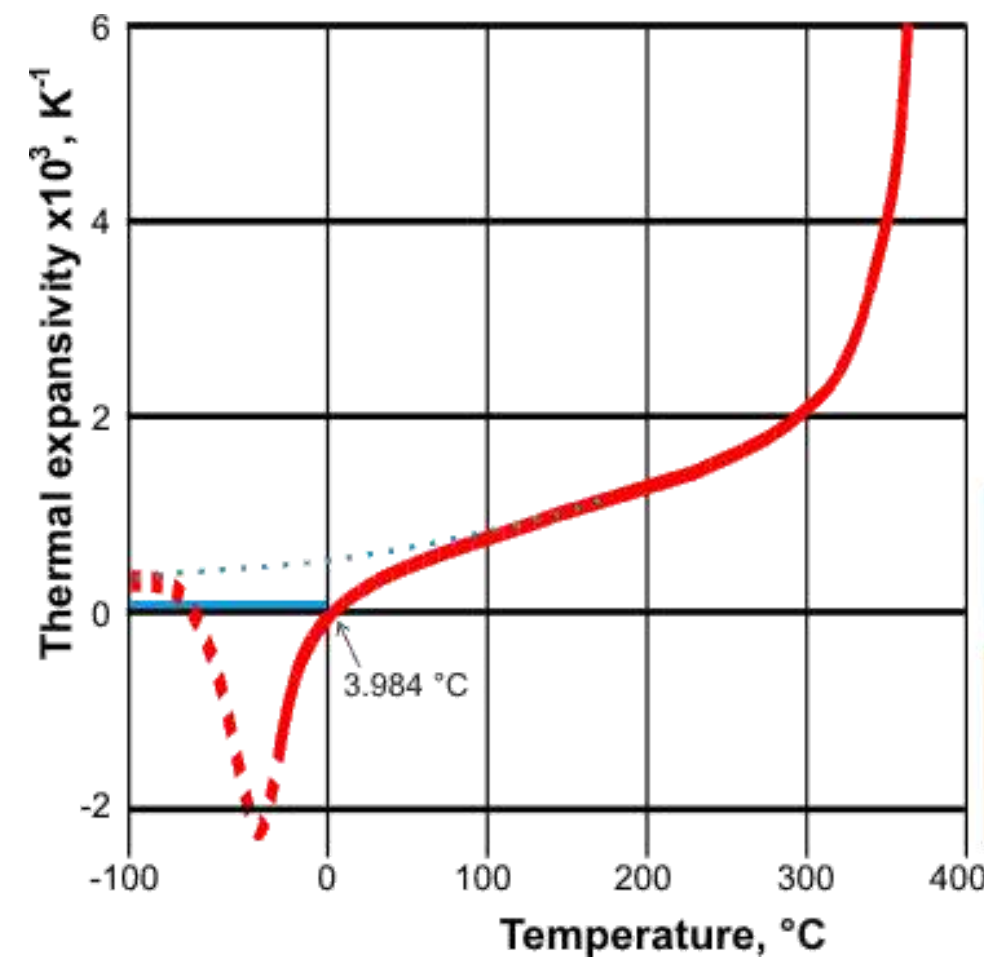
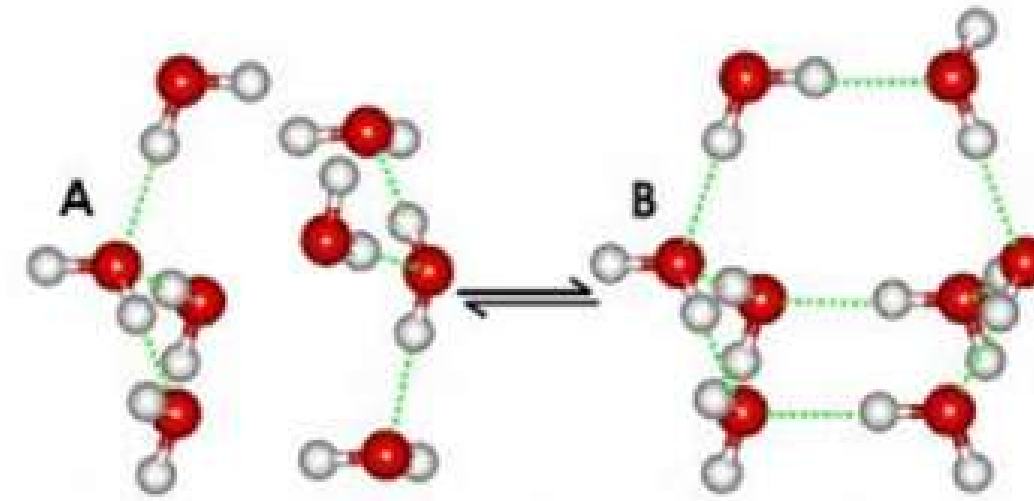
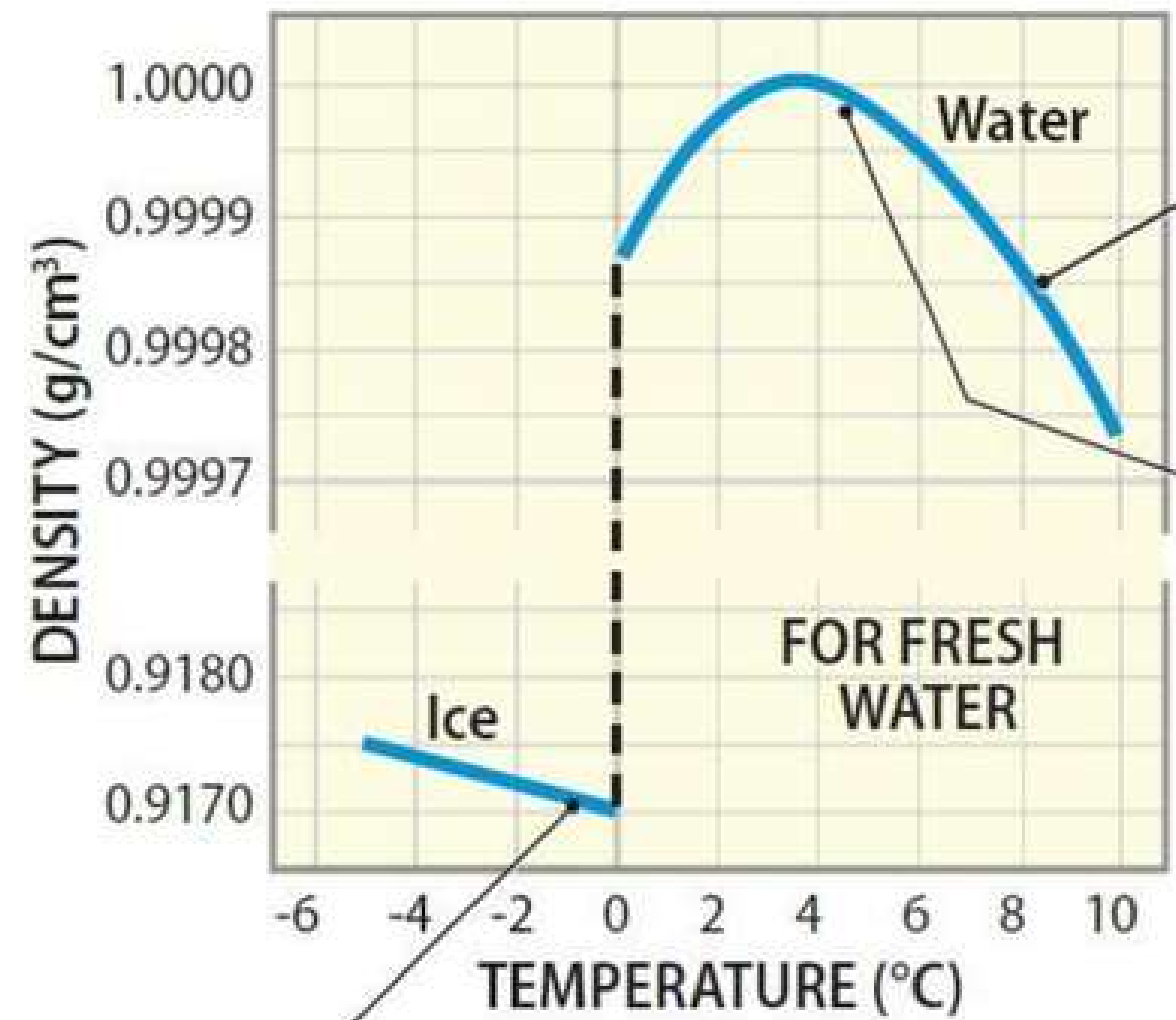
https://water.lsbu.ac.uk/water/martin_chaplin.html



water

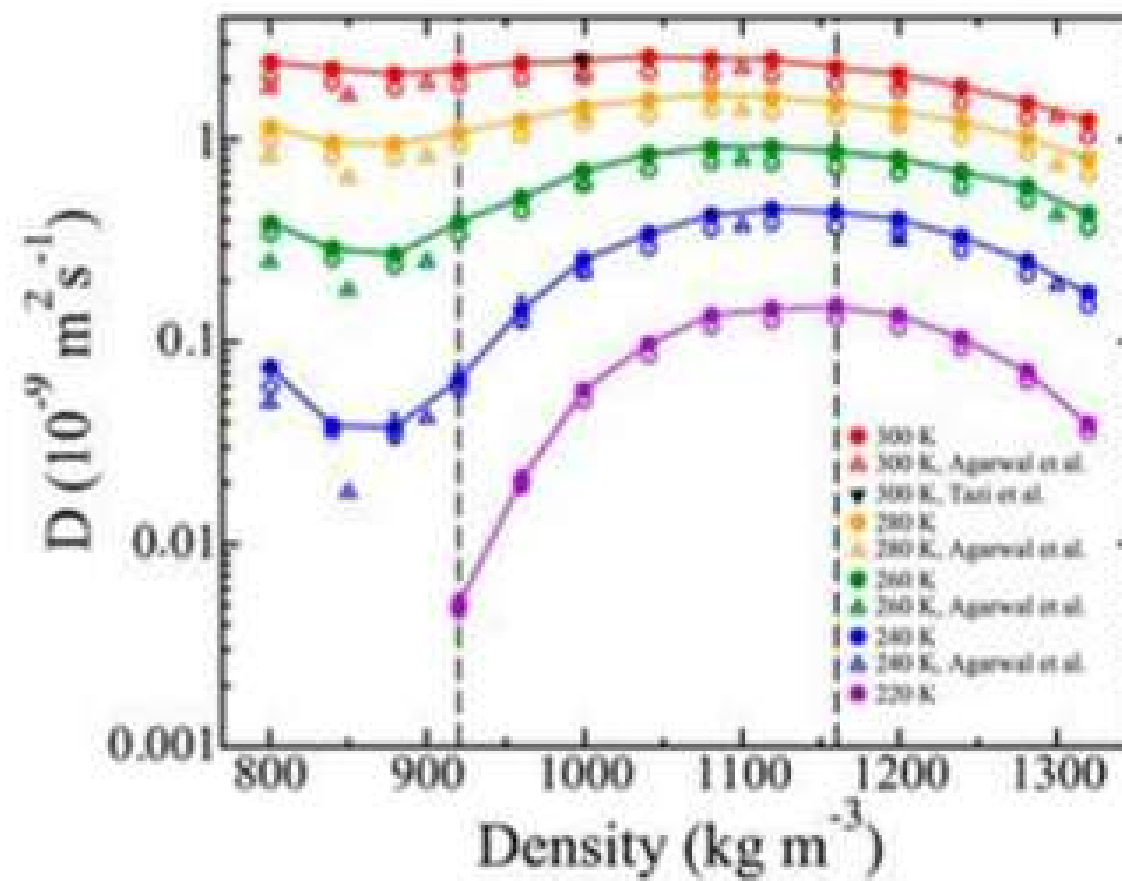


density is strange

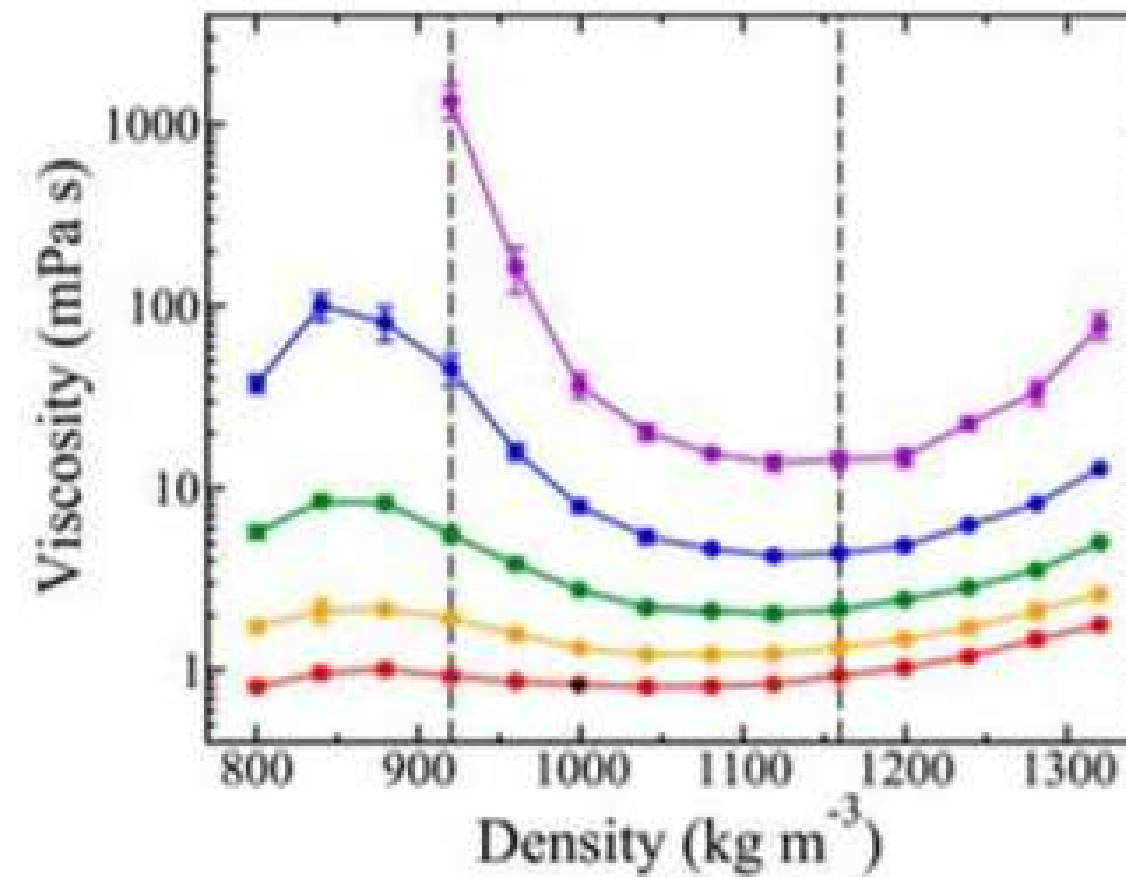


water

diffusion is strange



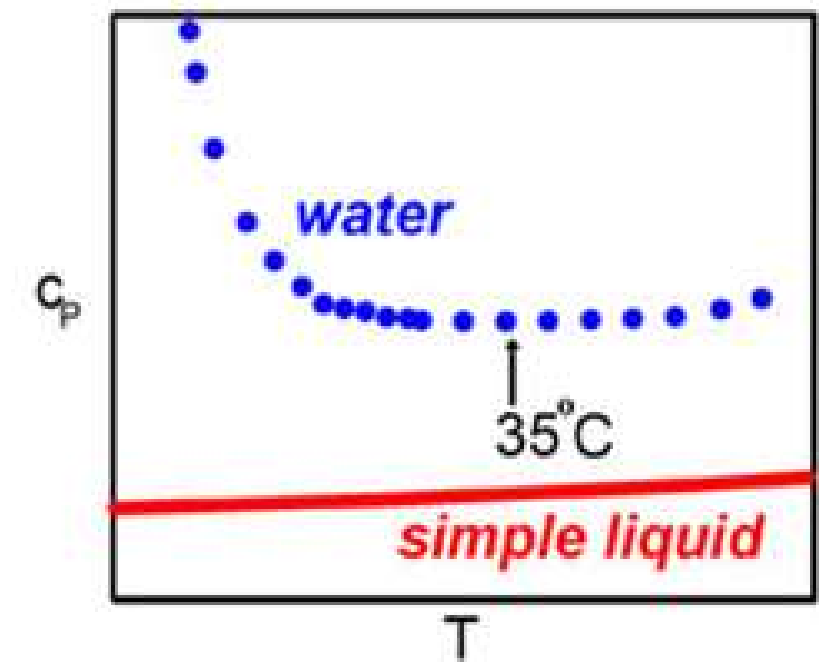
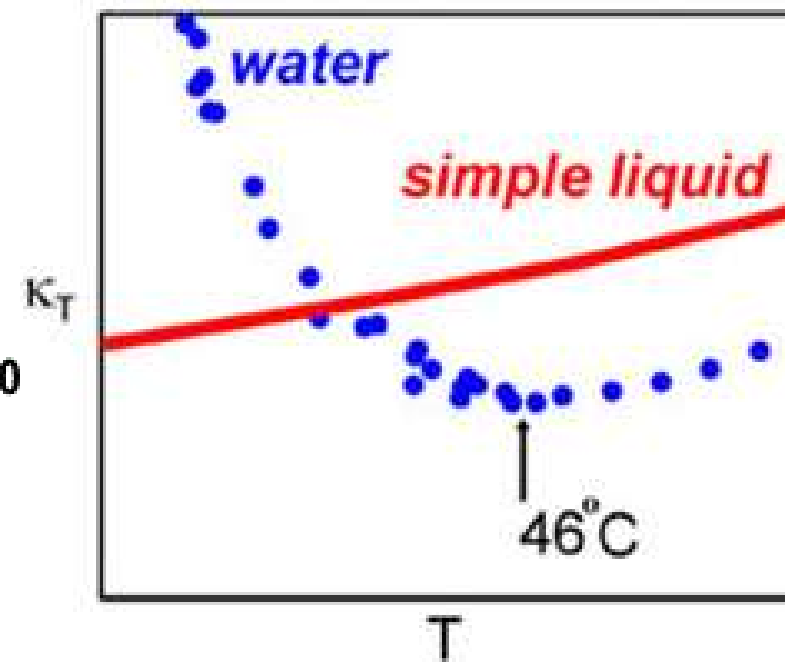
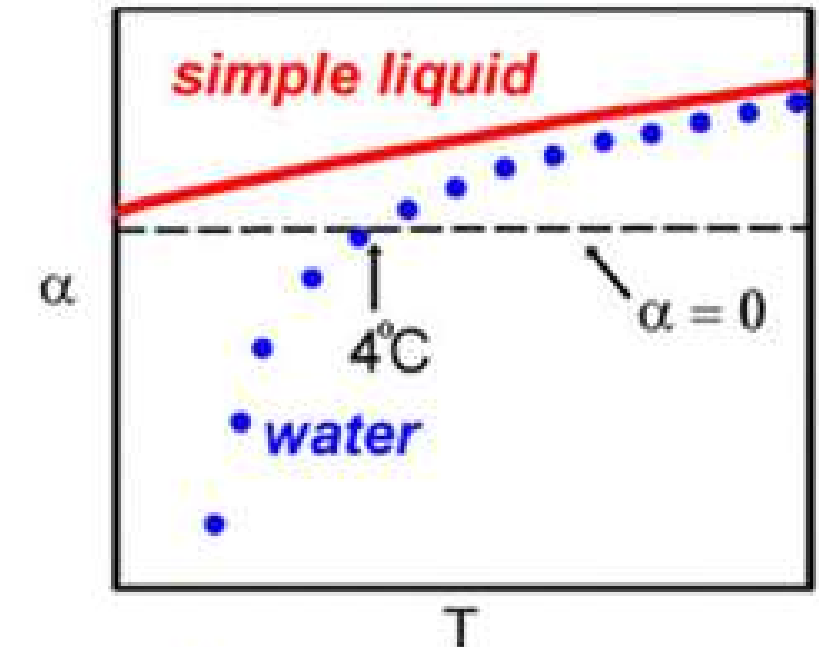
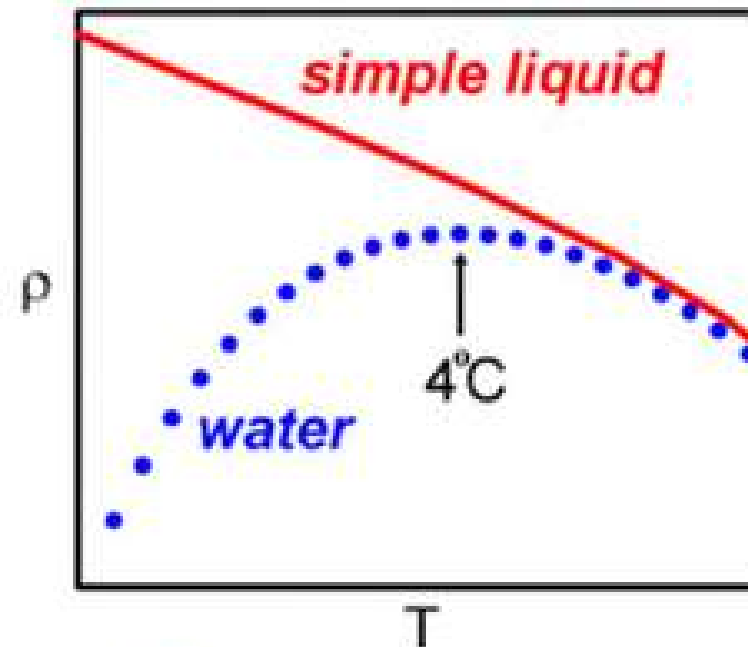
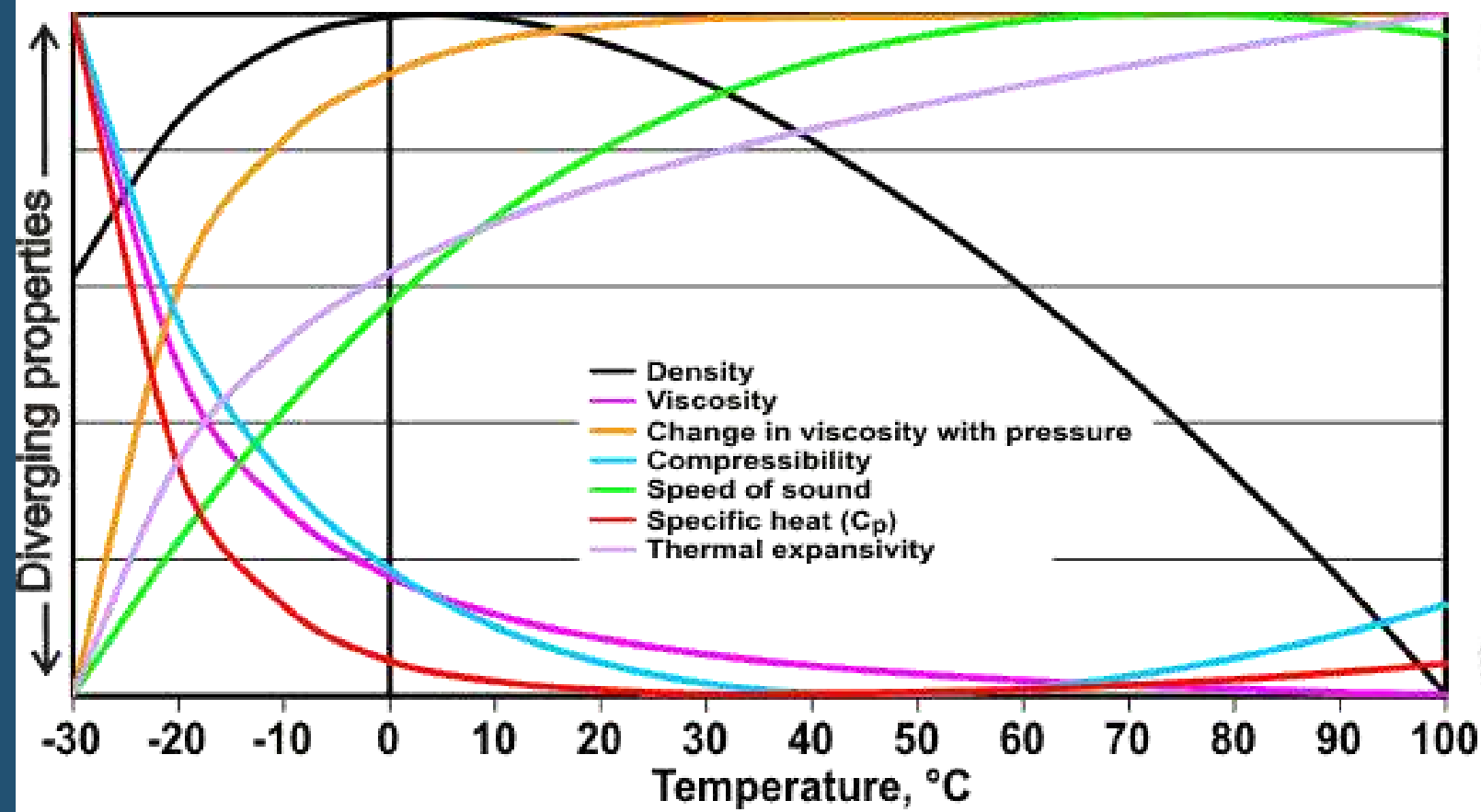
$$D = \frac{kT}{6\pi\eta R}$$



de Hijes et al, J. Chem. Phys. **149**, 094503 (2018)

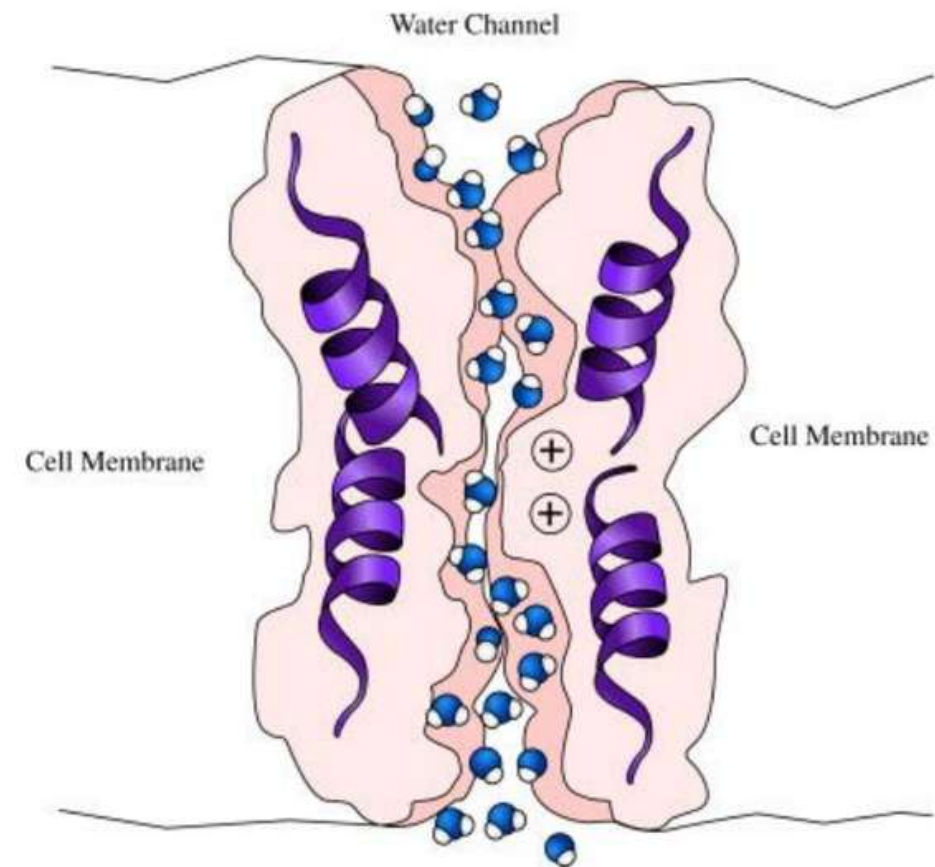
water

is really strange

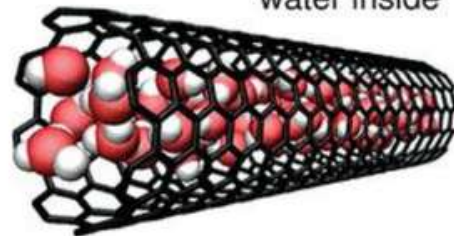


water

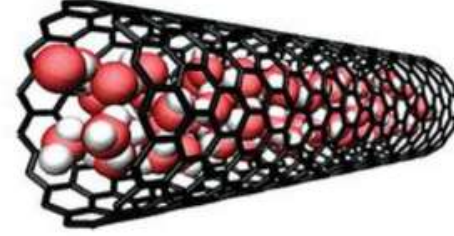
in nanoconfinement is strange



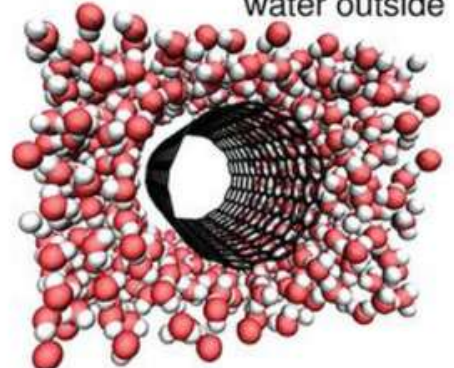
a) armchair CNT – water inside



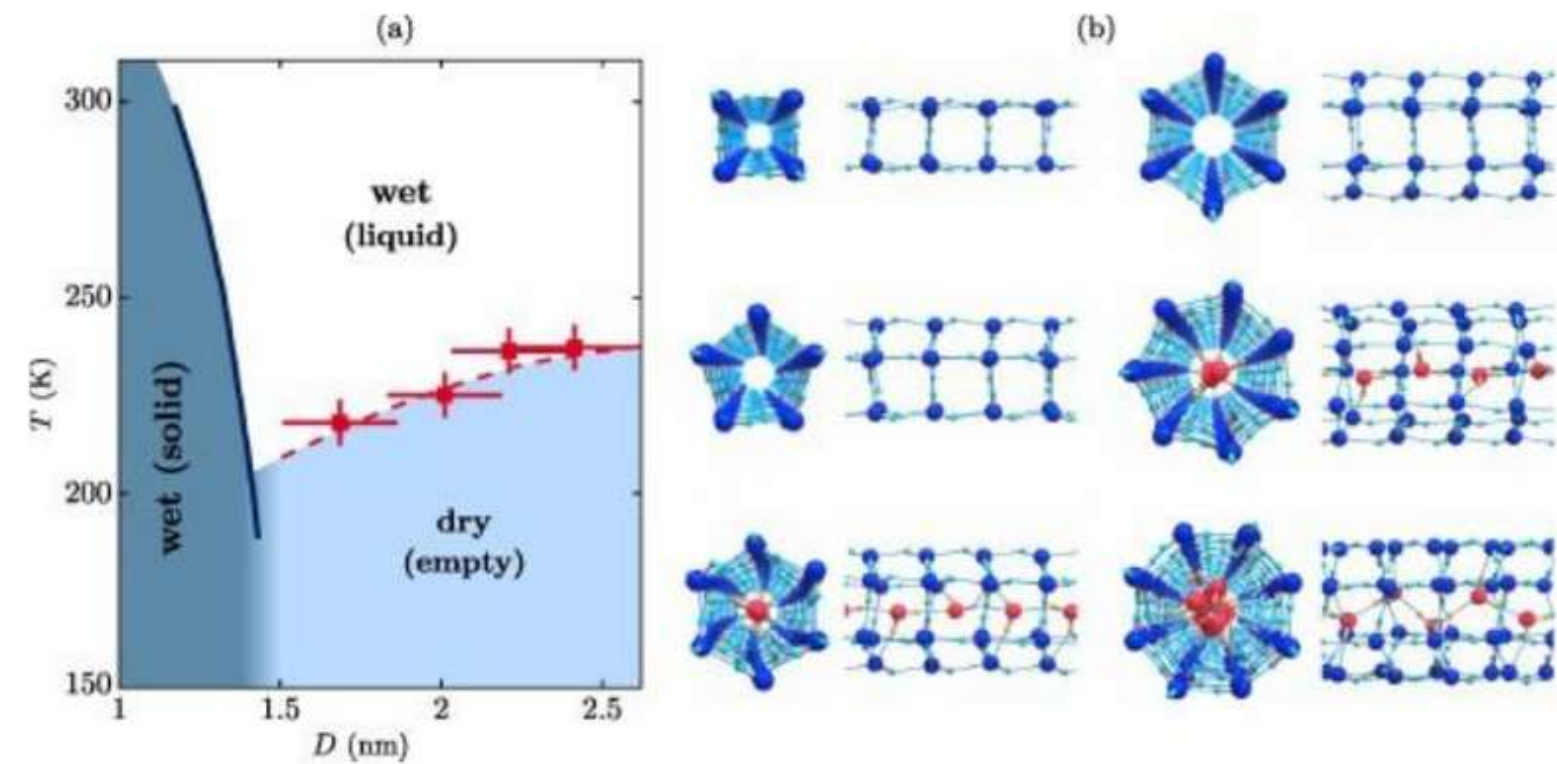
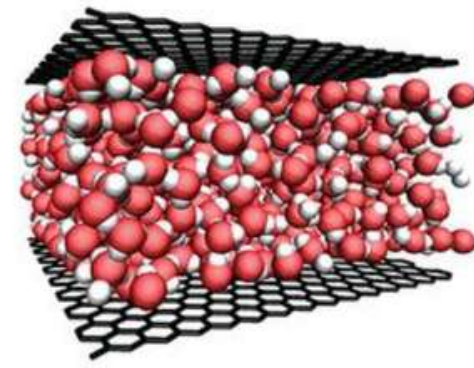
b) zigzag CNT



c) armchair CNT – water outside



d) graphene planes



Mochizuki, K., Koga, K., 2015. Proc. Natl. Acad. Sci. USA 112, 8221–8226

water

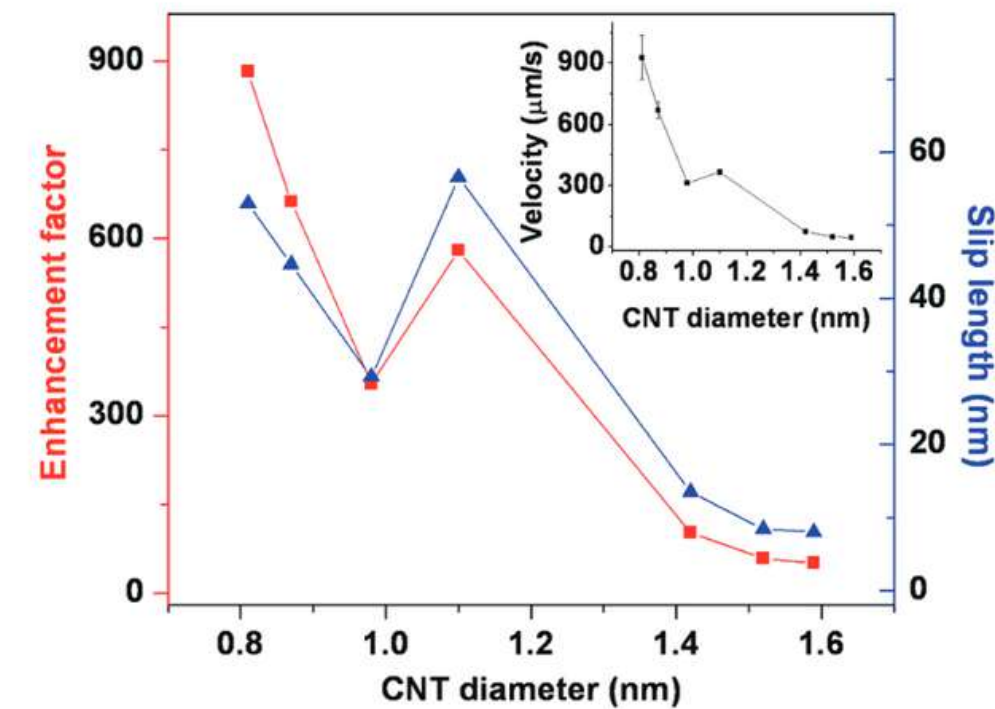
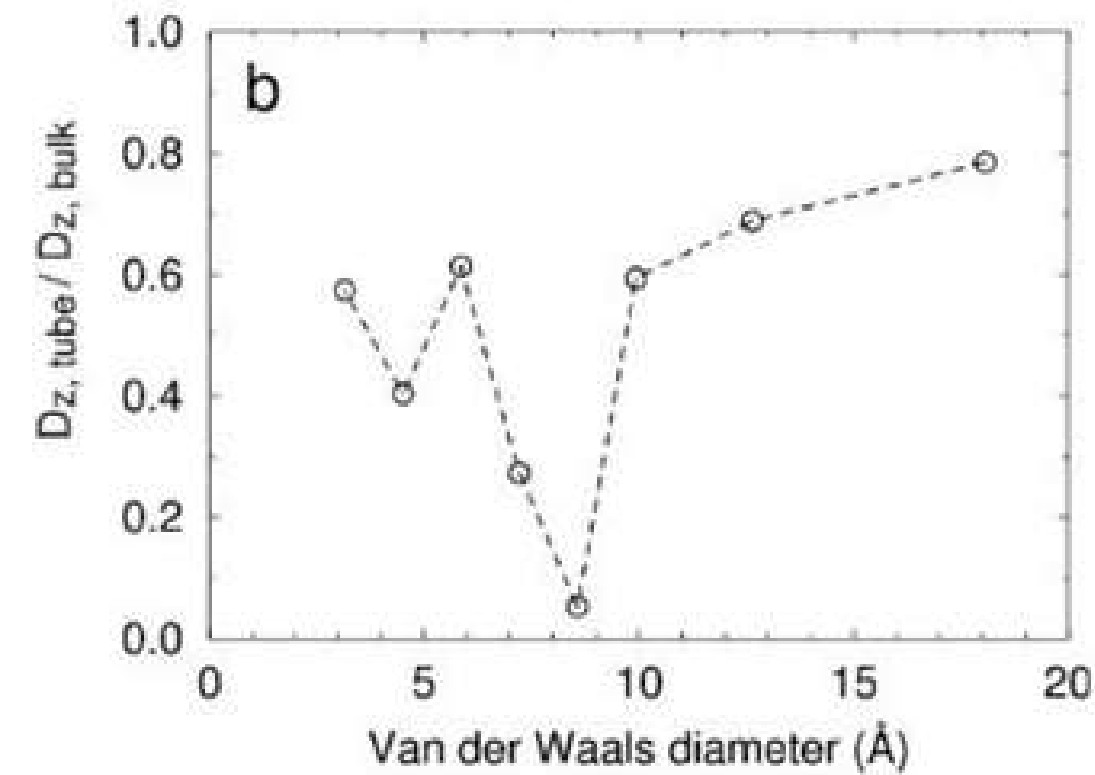
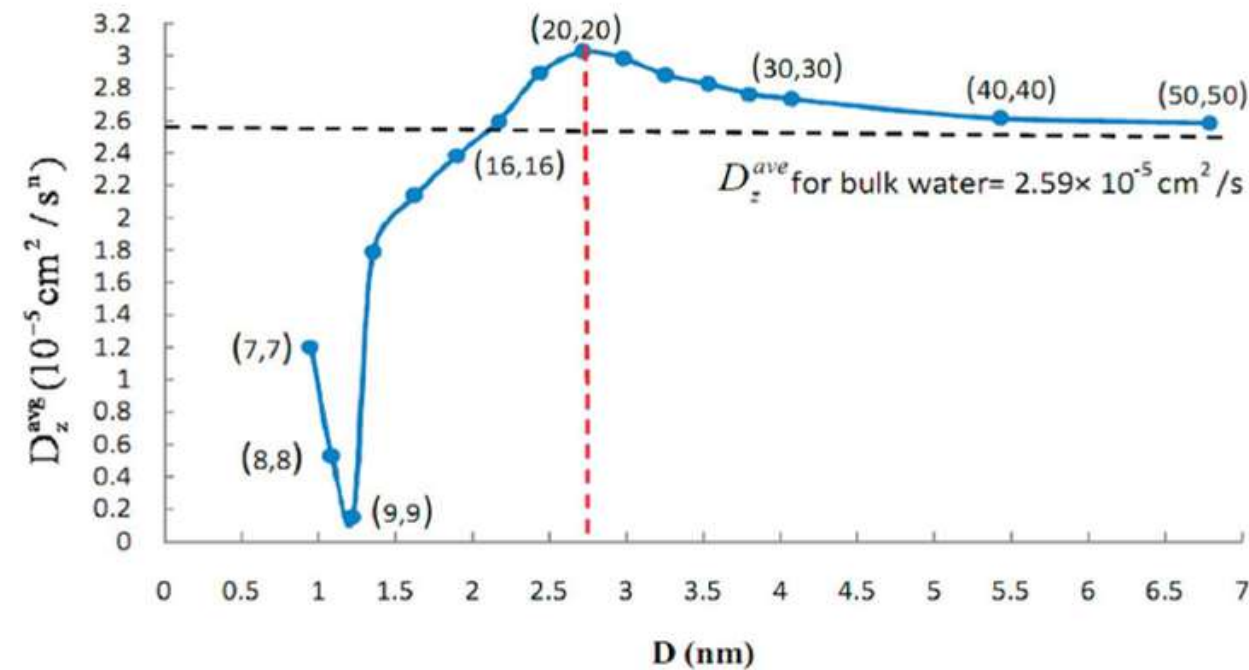
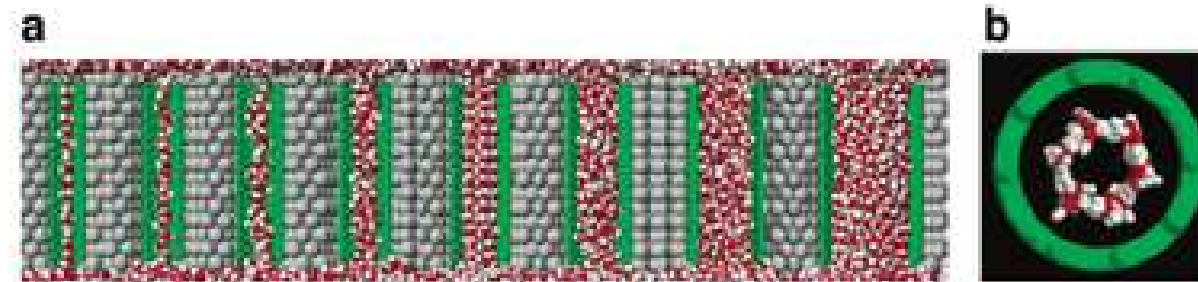
in nanoconfinement is strange



Anomalous Immobilized Water: A New Water Phase Induced by Confinement in Nanotubes

R. Jay Mash, ^{1,2,3} Somy Joseph, ¹ N. R. Aluru, ^{1,2,3,4} and Eric Jakobsson ^{1,2,3,4}

NANO
LETTERS
2003
Vol. 3, No. 5
589–592



Farimani e Aluru, *J. Phys. Chem. B* 2011, 115, 42, 12145–12149

QIN ET AL. *NANO LETT.* 2011, 11, 5, 2173–2177

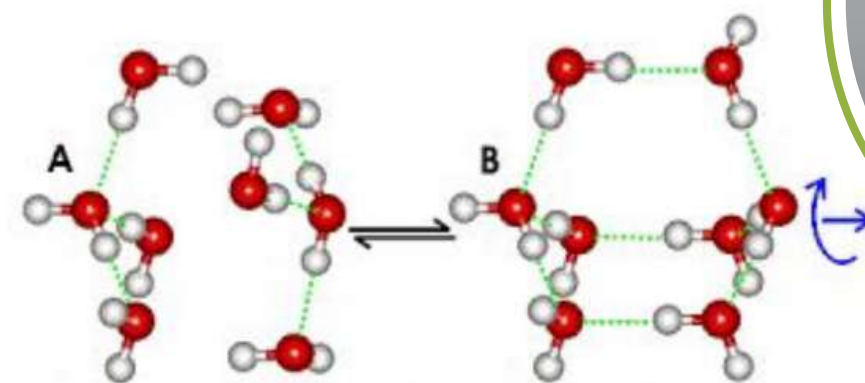
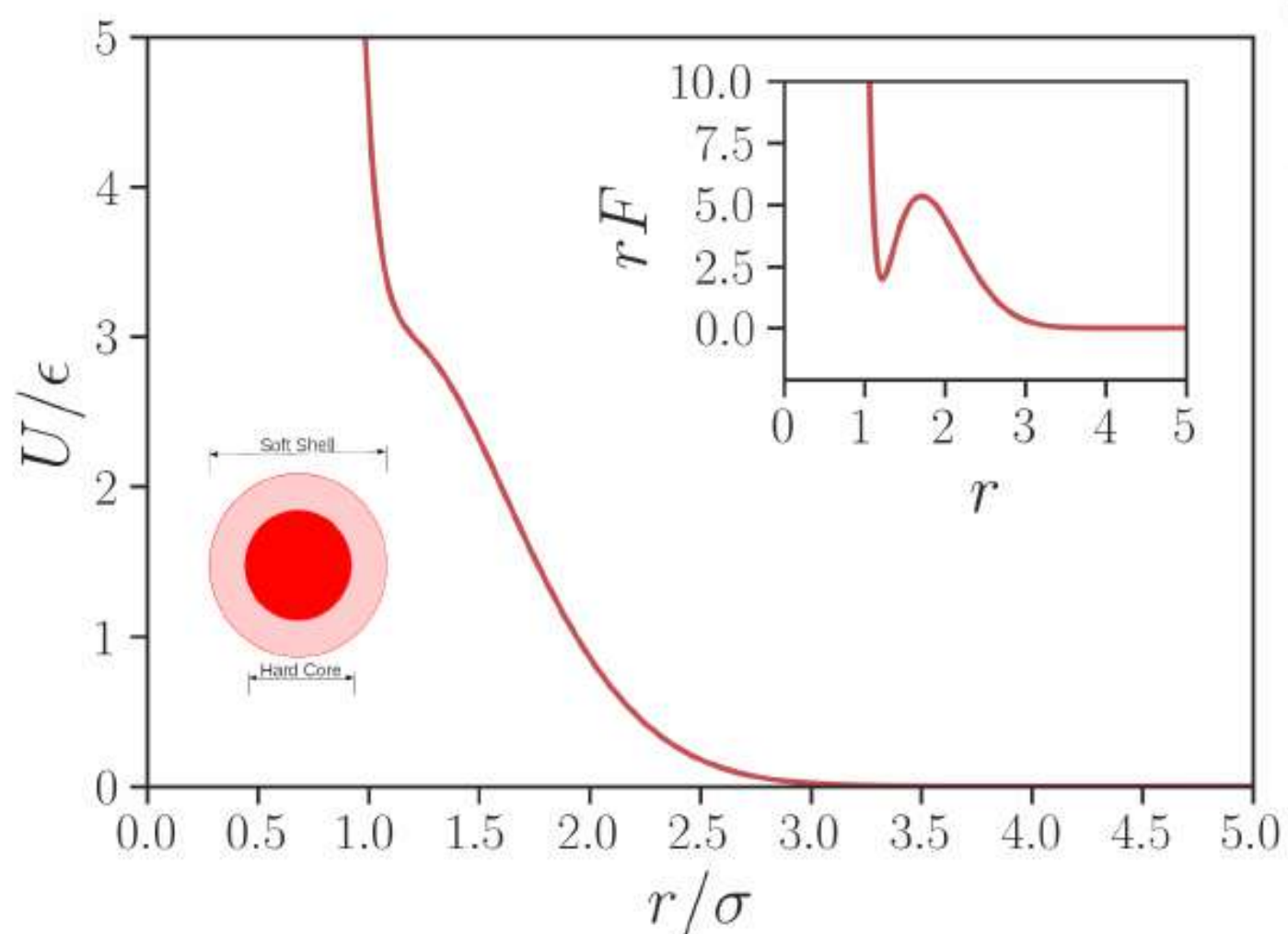
WATER AT NANOSCALE

CS “water” is strange

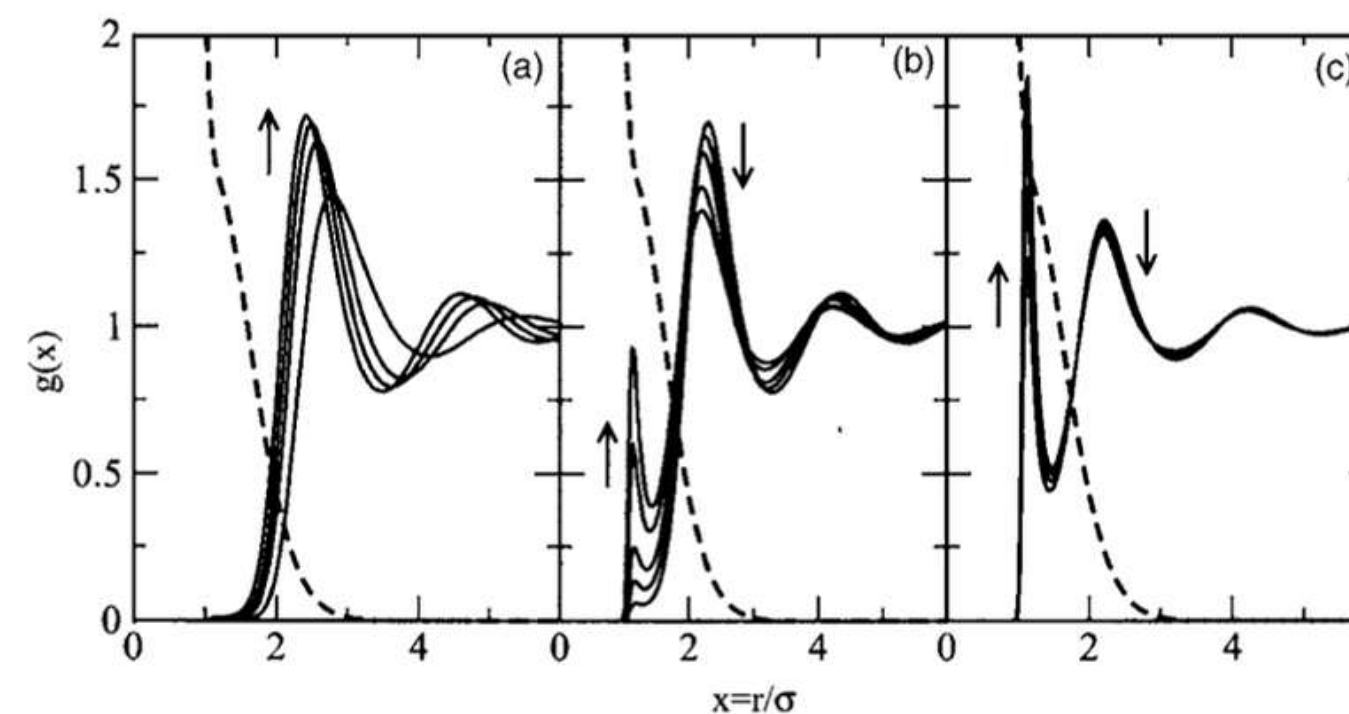
Thermodynamic and dynamic anomalies for a three-dimensional isotropic core-softened potential

Alan Barros de Oliveira, Paulo A. Netz, Thiago Colla, and Marcia C. Barbosa

Citation: *J. Chem. Phys.* **124**, 084505 (2006); doi: 10.1063/1.2168458



MARCIA BARBOSA
GRUPO DE FLUIDOS
COMPLEXOS (UFRGS)



CS “water”



in nanoconfinement is strange?



Thermodynamic and dynamic anomalies for a three-dimensional isotropic core-softened potential

Alan Barros de Oliveira, Paulo A. Netz, Thiago Colla, and Marcia C. Barbosa

Citation: *J. Chem. Phys.* **124**, 084505 (2006); doi: 10.1063/1.2168458

The Journal of
Chemical Physics

RESEARCH ARTICLE | APRIL 03 2023

Solid-amorphous transition is related to the waterlike anomalies in a fluid without liquid–liquid phase transition

FREE

J. R. Bordin and L. B. Krott

Special Collection: 2023 JCP Emerging Investigators Special Collection

José Rafael Bordin ; Leandro B. Krott

Check for updates

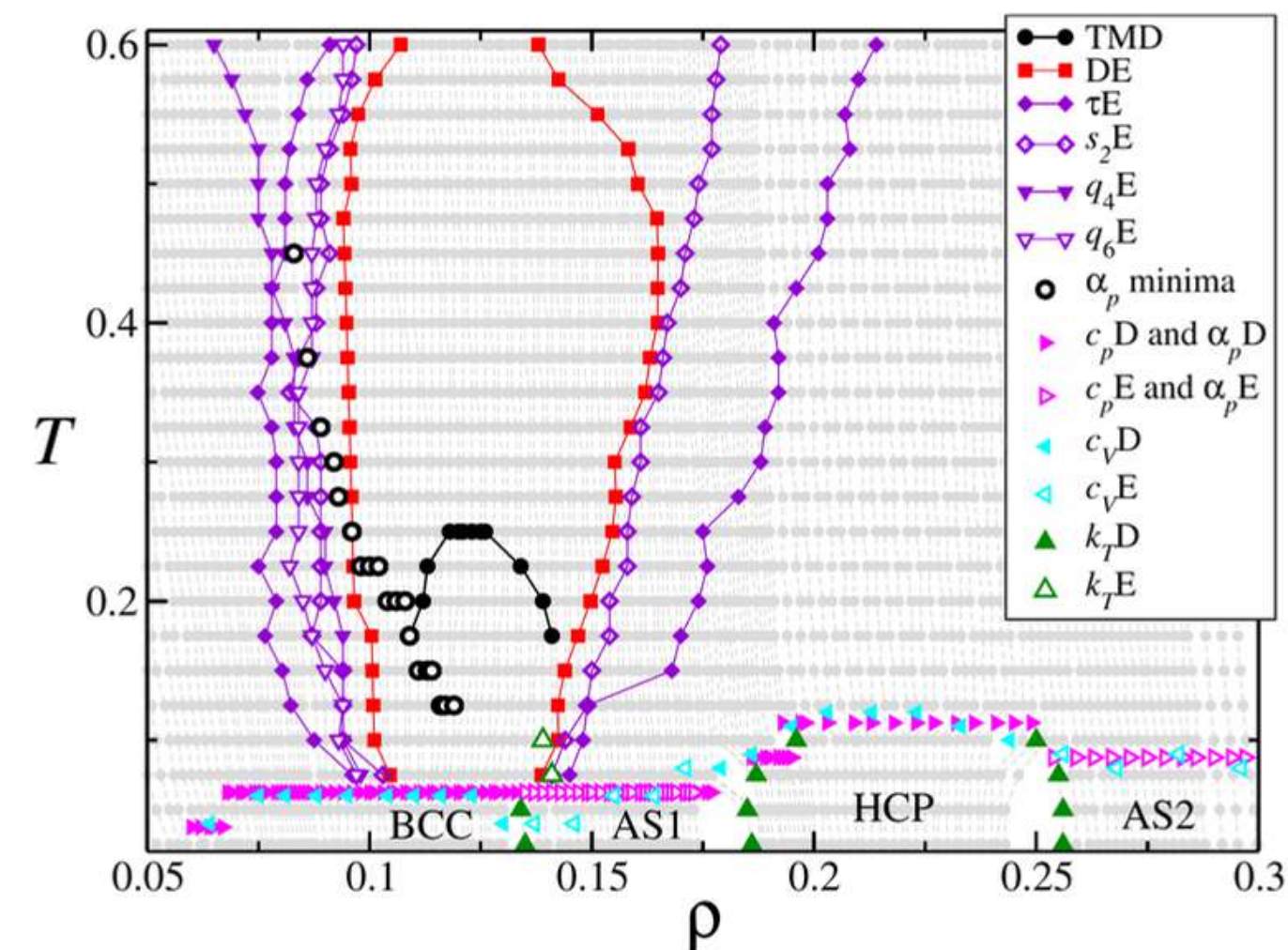
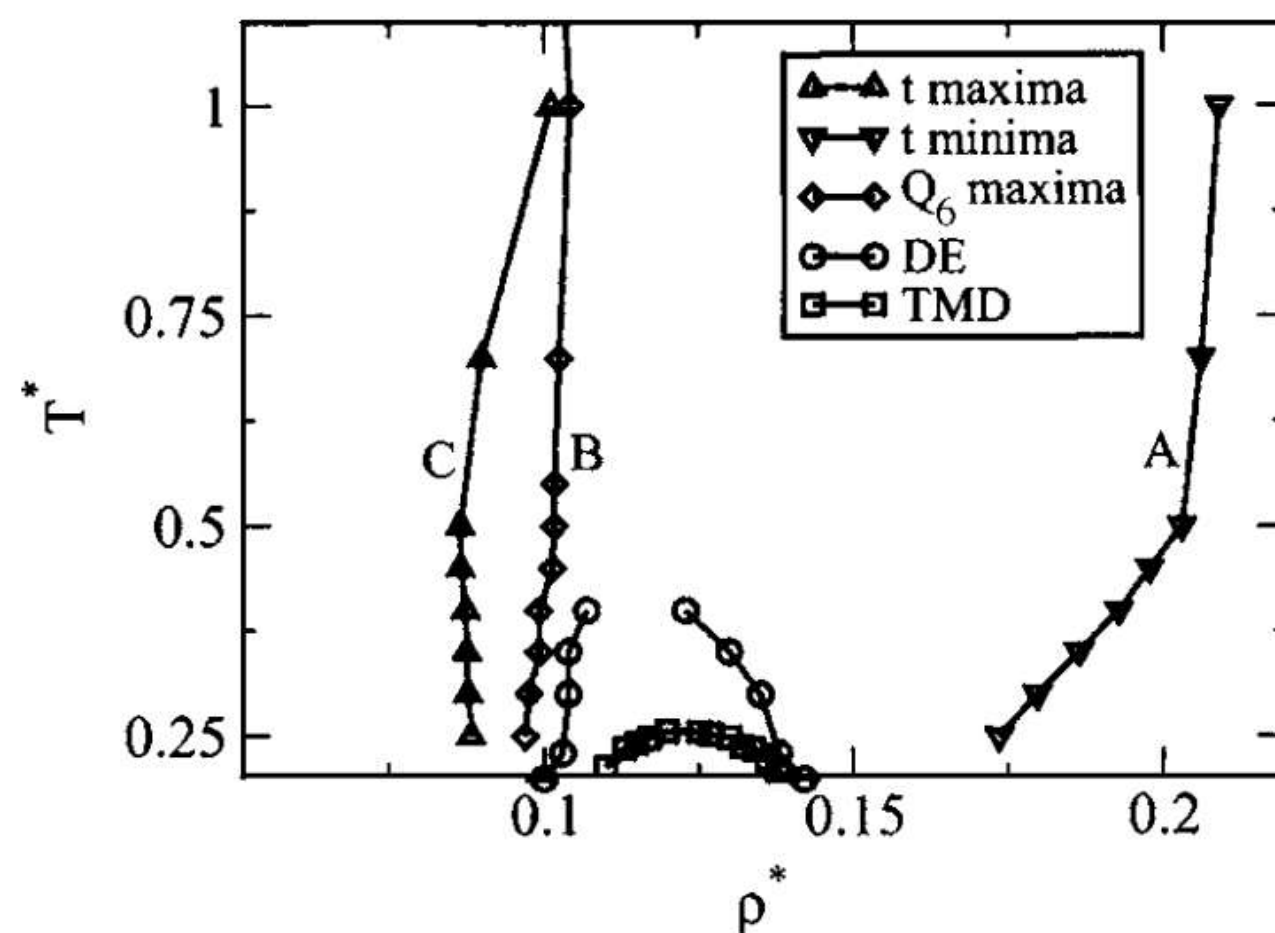
J. Chem. Phys. **158**, 134501 (2023)

<https://doi.org/10.1063/5.0144868>

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Online

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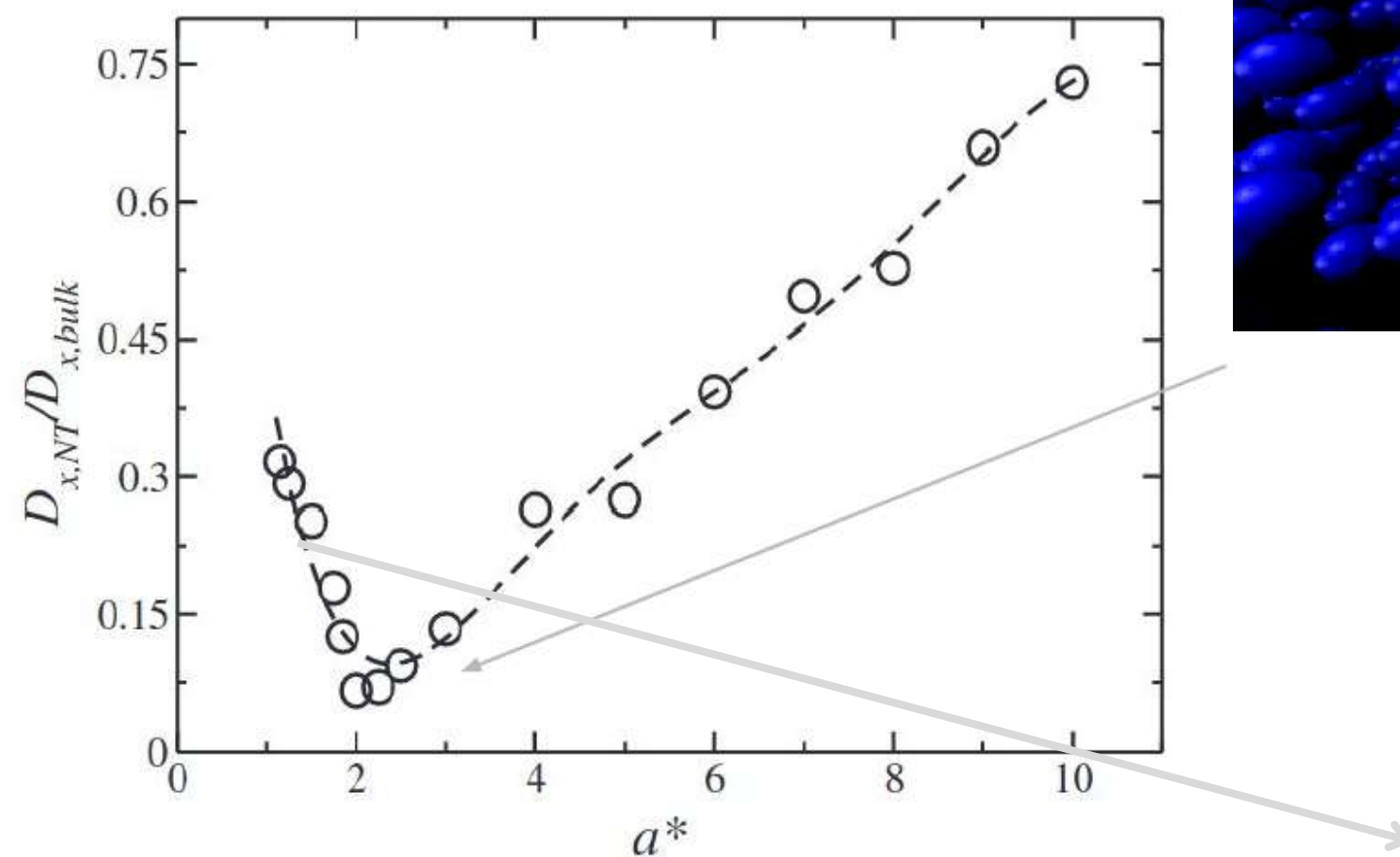


WATER AT NANOSCALE

CS “water”



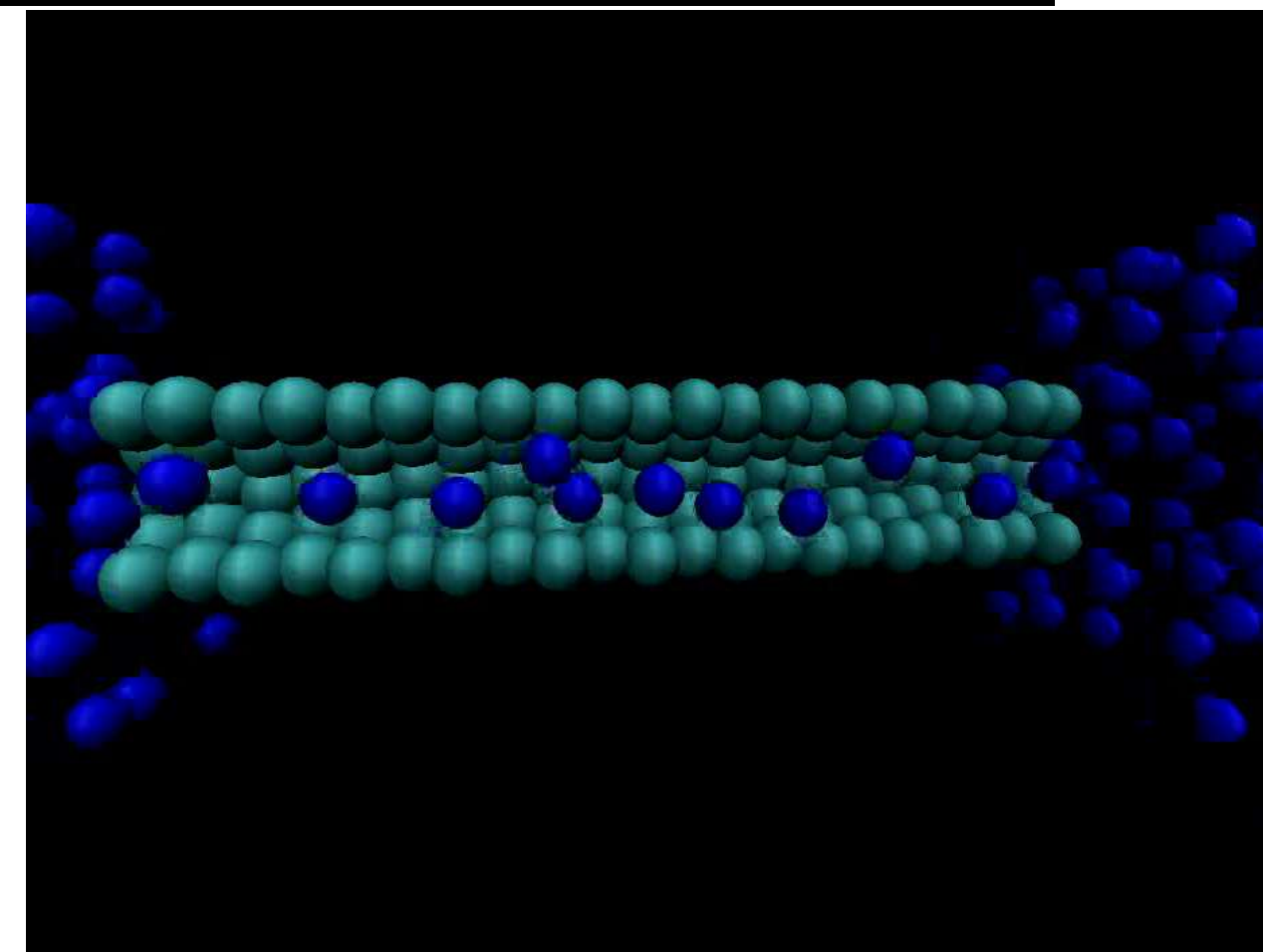
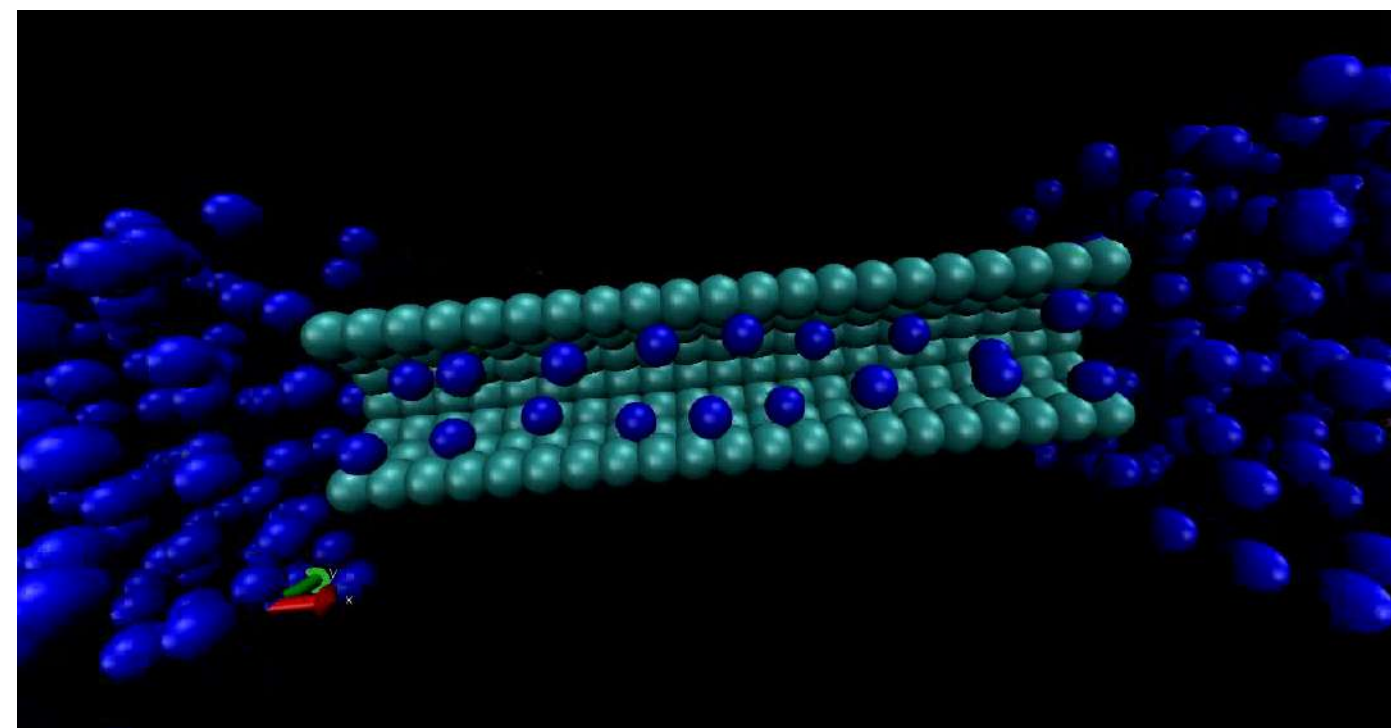
in nanoconfinement is strange!!

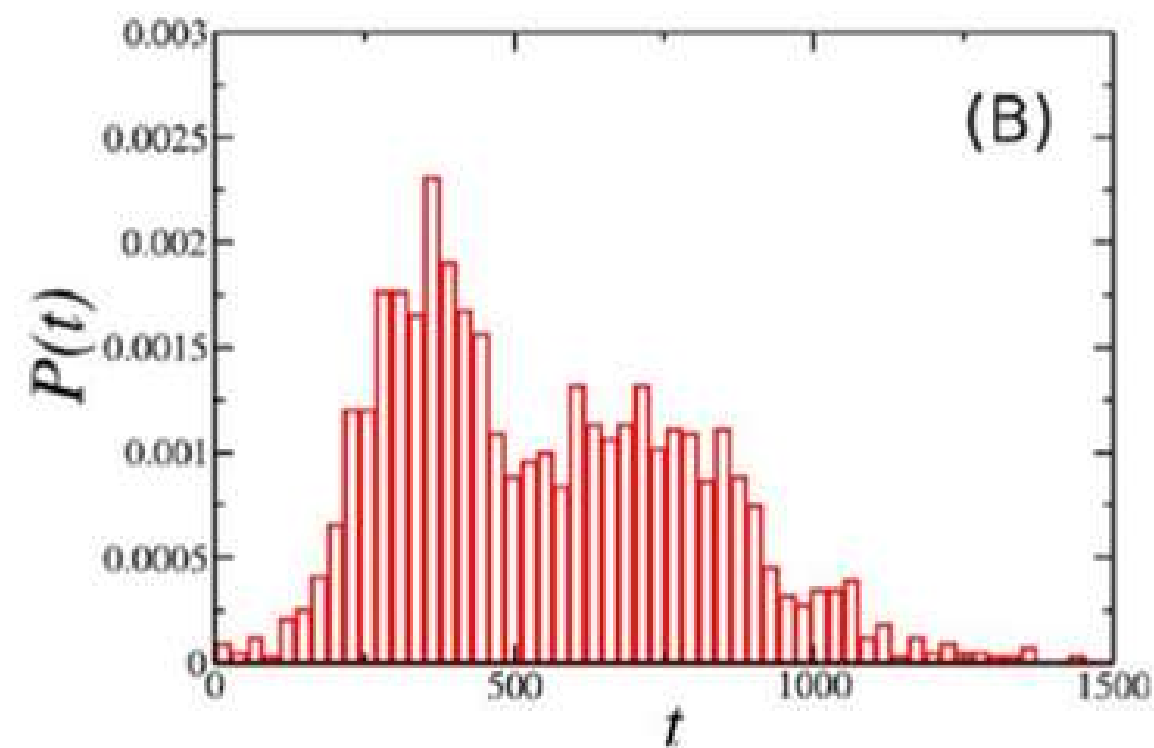
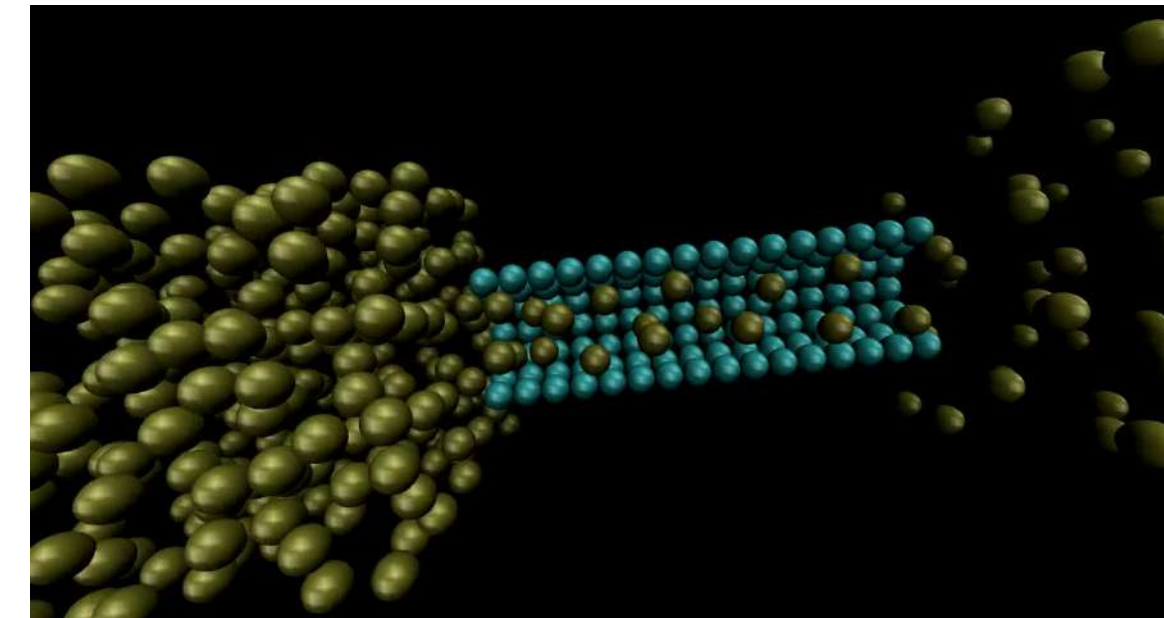


THE JOURNAL OF CHEMICAL PHYSICS **137**, 084504 (2012)

Diffusion enhancement in core-softened fluid confined in nanotubes

J. R. Bordin,^{1,a)} A. B. de Oliveira,^{2,b)} A. Diehl,^{3,c)} and Marcia C. Barbosa^{4,d)}



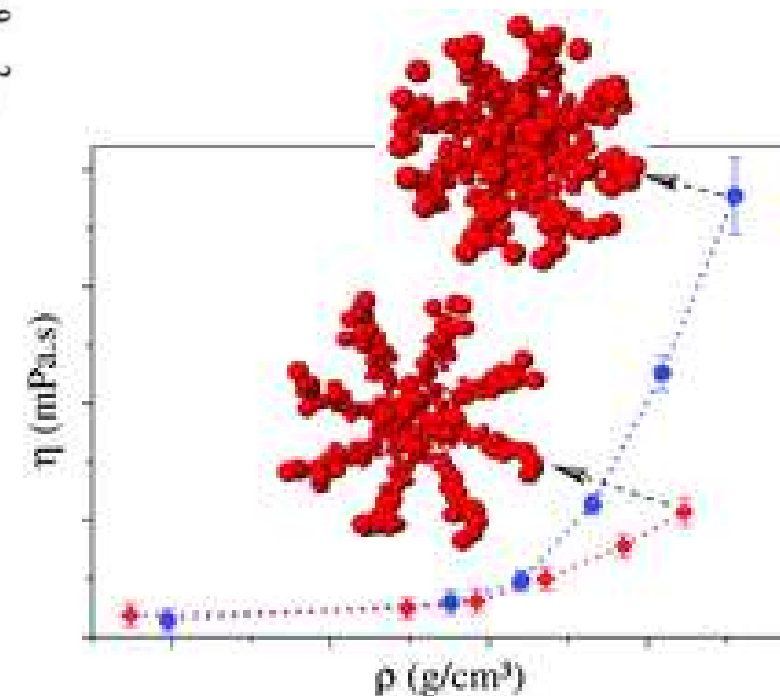
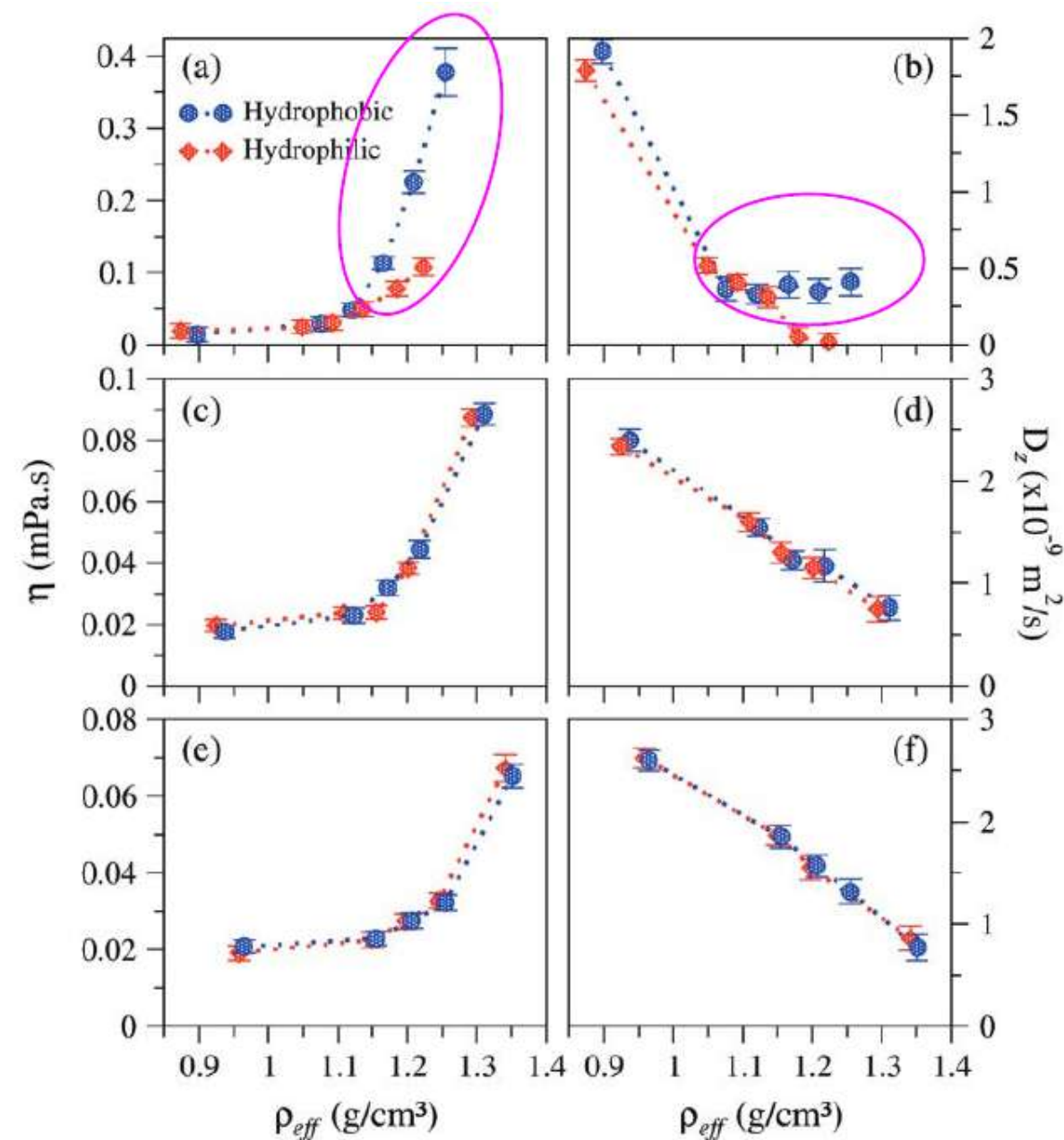
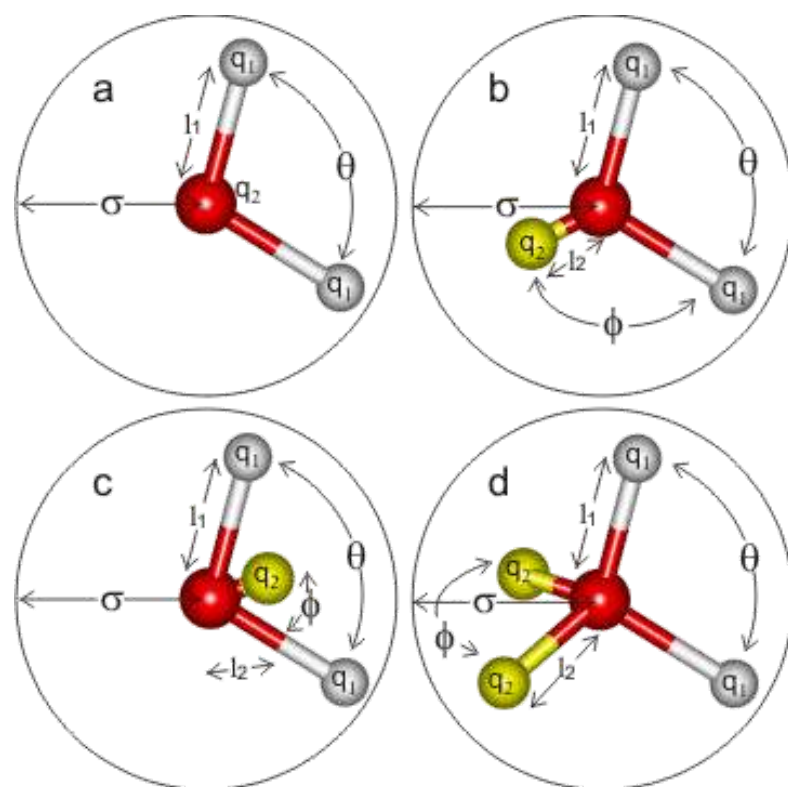


Volume 1 Number 1 February 2004





MATEUS H. KÖHLER
LABORATÓRIO
COMPUTACIONAL DE
NANOMATERIAIS (UFMS)



PCCP

PAPER



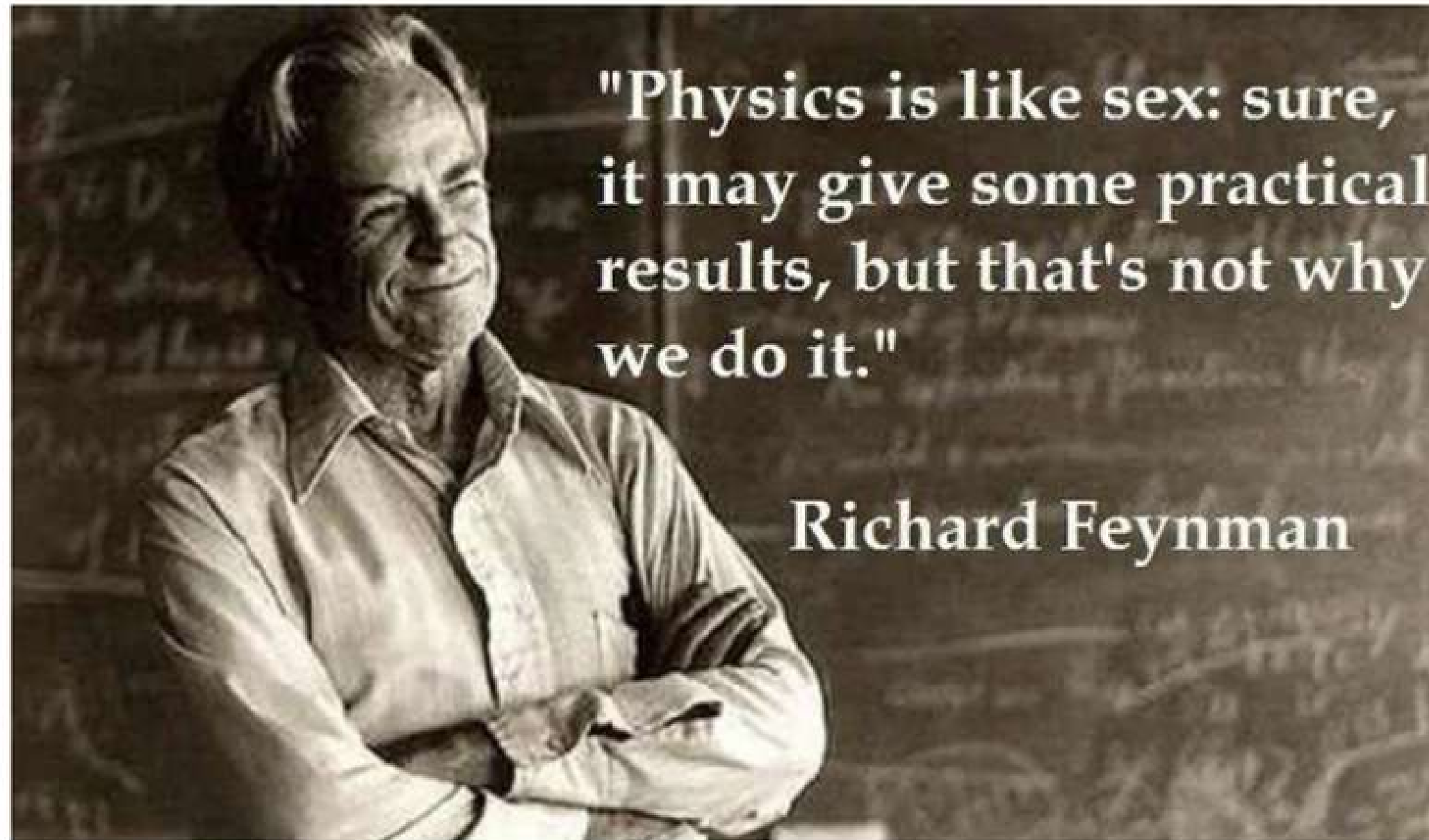
Cite this: *Phys. Chem. Chem. Phys.*,
2017, 19, 12921

Breakdown of the Stokes–Einstein water transport through narrow hydrophobic nanotubes

Mateus Henrique Köhler,^a José Rafael Bordin,^b Leandro B. da Silva^c and
Marcia C. Barbosa^a



View Article Online
View Journal | View Issue

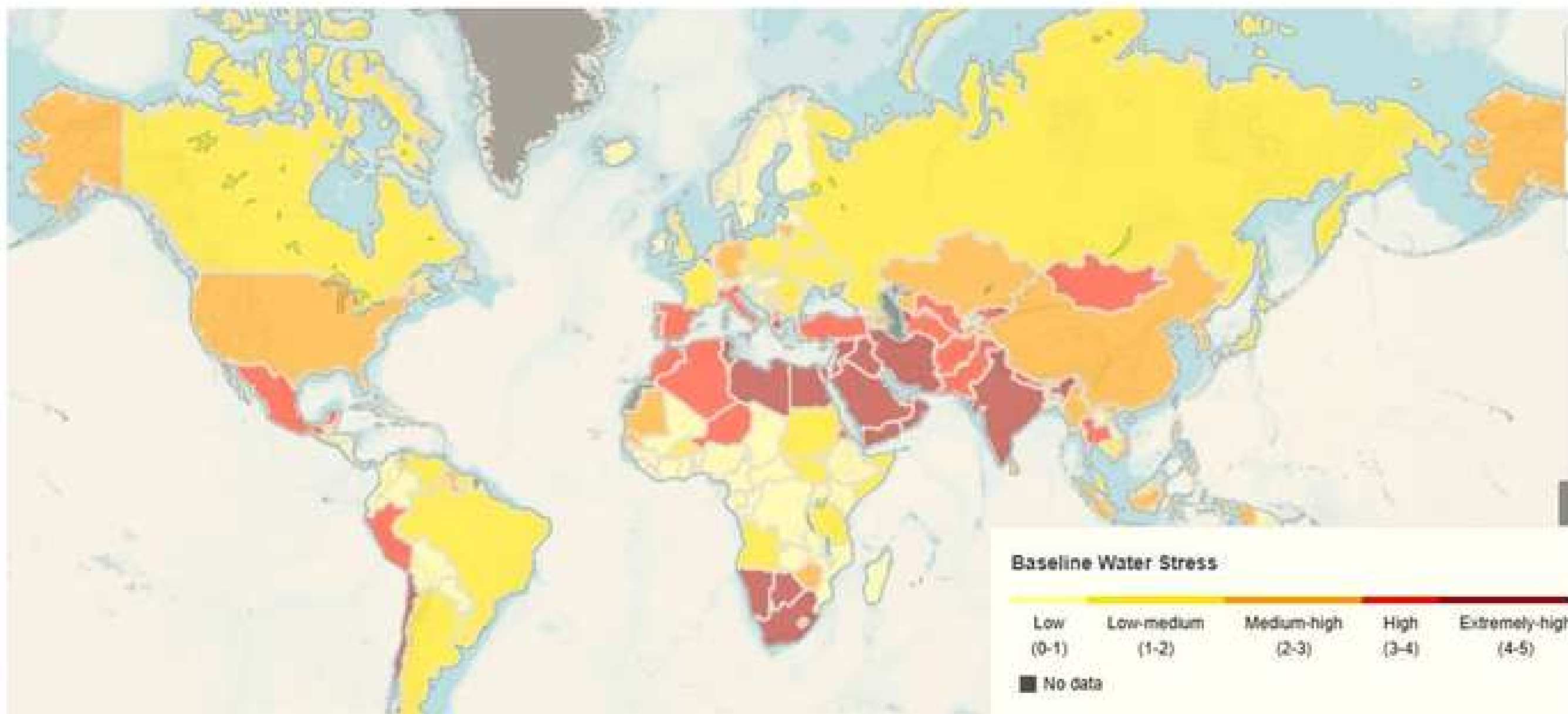






O estresse hídrico no mundo

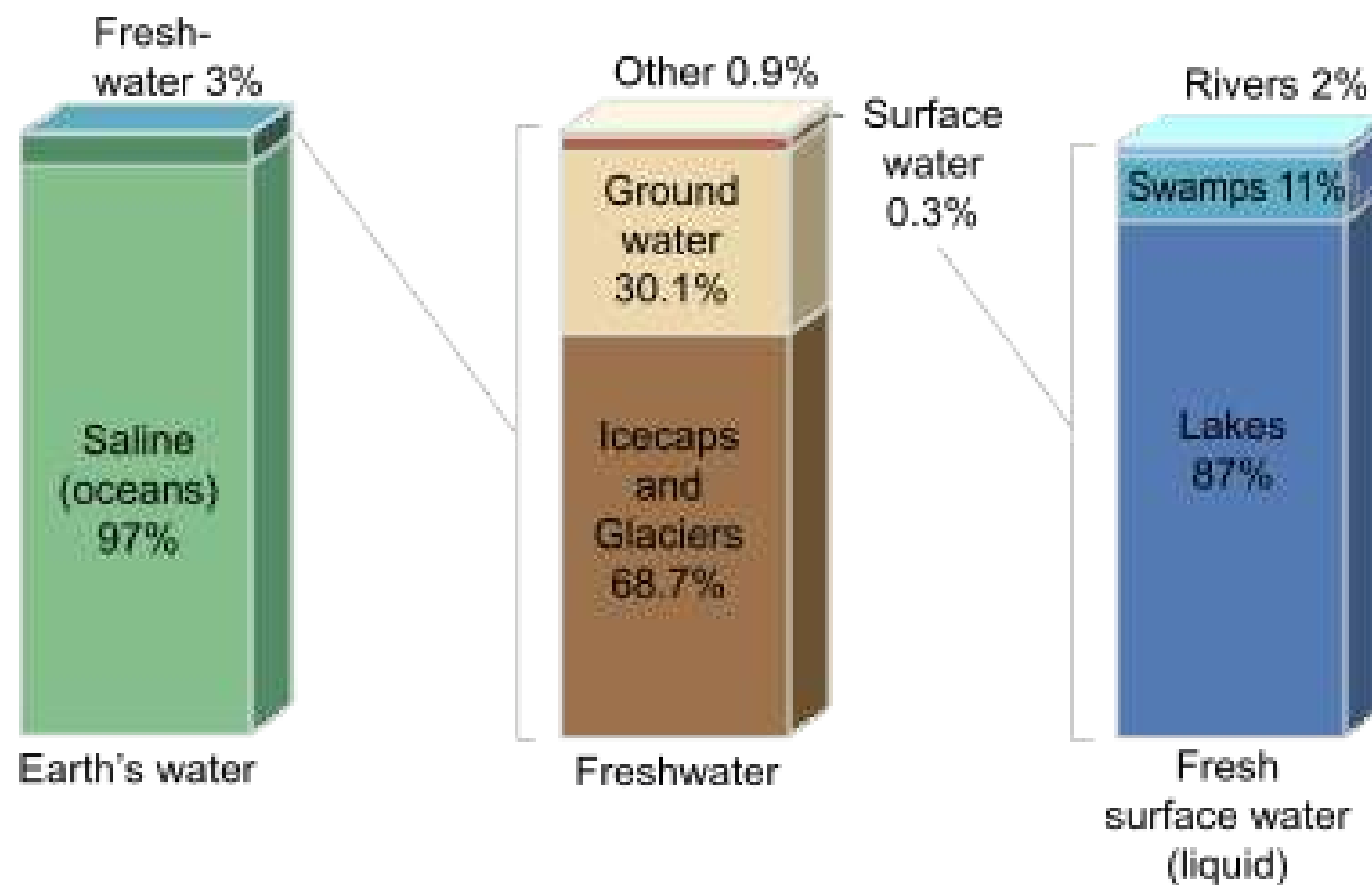
25 países estão expostos atualmente a "estresse hídrico extremo". Um país que enfrenta "estresse hídrico extremo" está usando pelo menos 80% de seu suprimento disponível.
A classificação "alto estresse hídrico" significa que o país está retirando 40% de seu suprimento



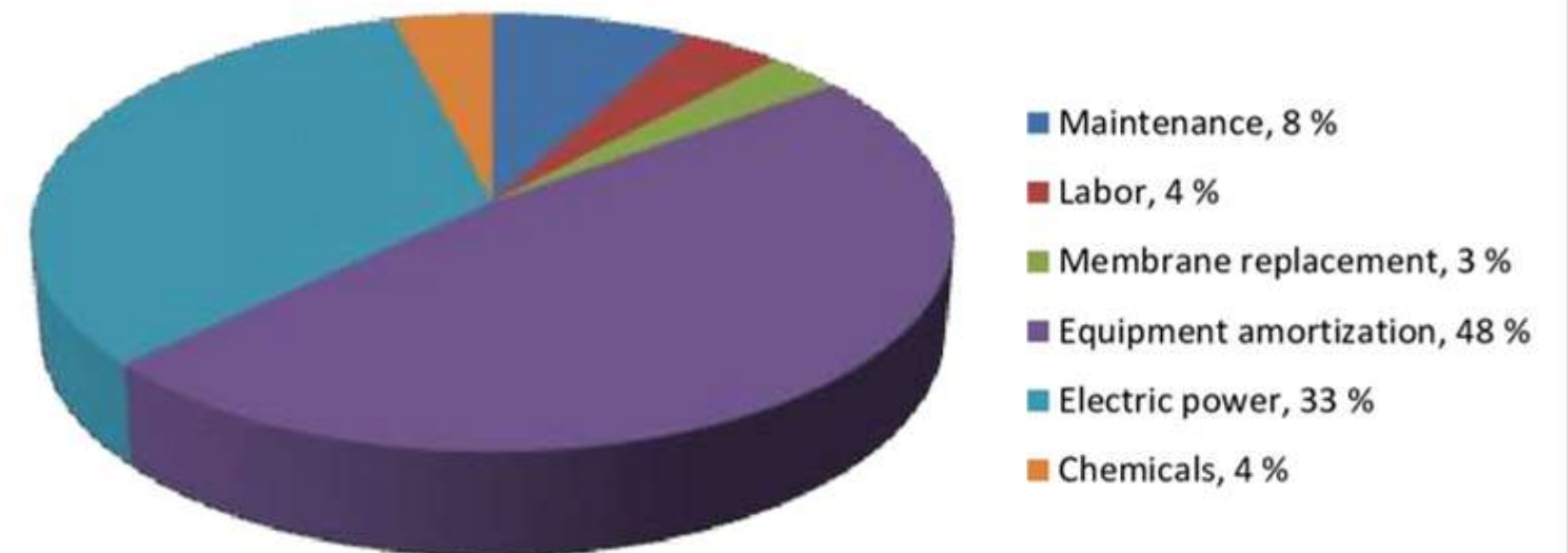
Fonte: World Resources Institute

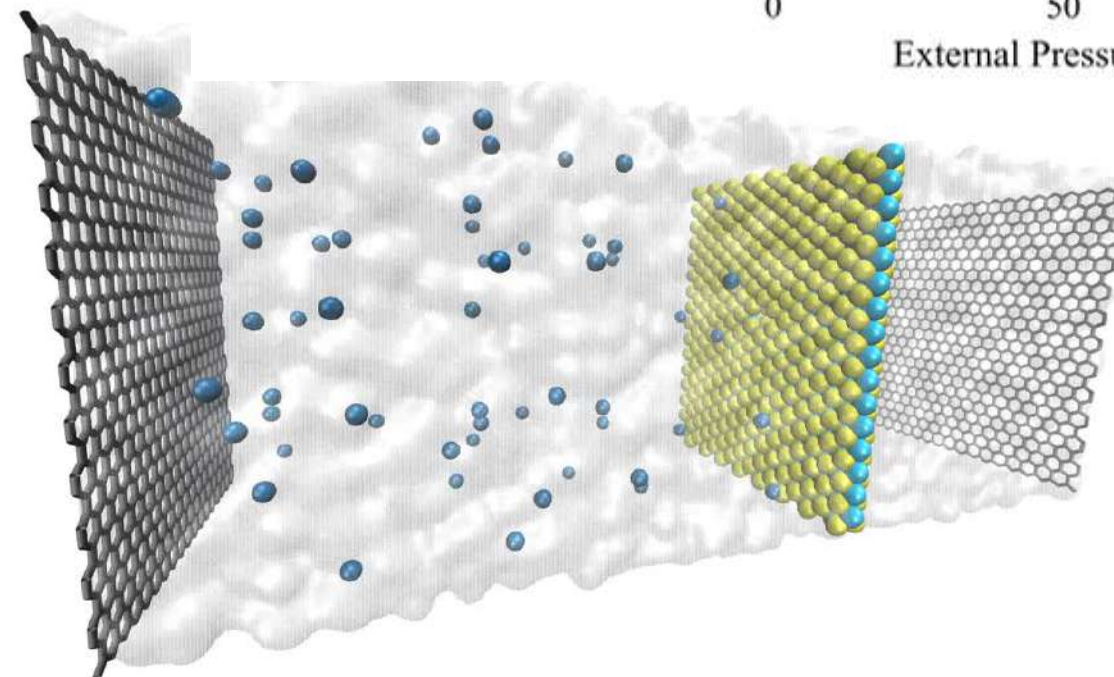
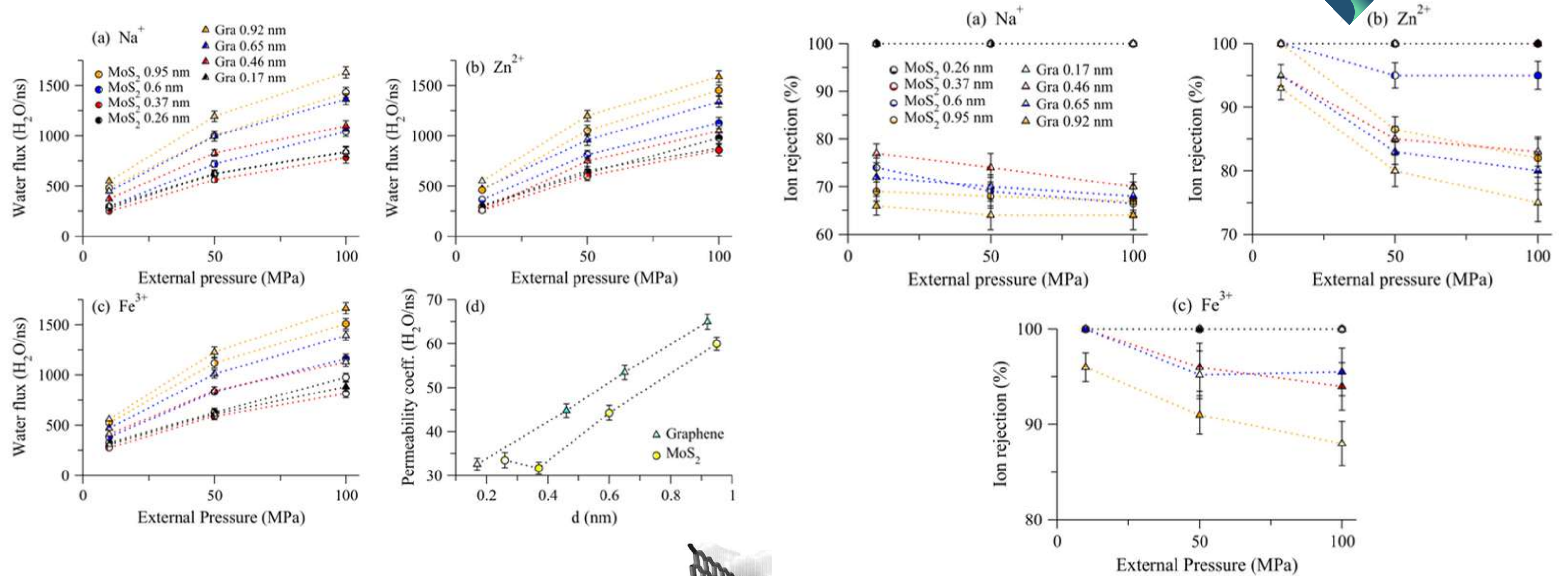


Distribution of Earth's Water



Costs (%)





RESEARCH ARTICLE | FEBRUARY 13 2018

2D nanoporous membrane for cation removal from water: Effects of ionic valence, membrane hydrophobicity, and pore size

Special Collection: [Ions in Water](#)

Mateus Henrique Köhler ; José Rafael Bordin ; Marcia C. Barbosa

Check for updates

J. Chem. Phys. 148, 222804 (2018)
<https://doi.org/10.1063/1.5013926>

Motivation

Contaminantes of Emerging Concern

EMERGING CONTAMINANTS



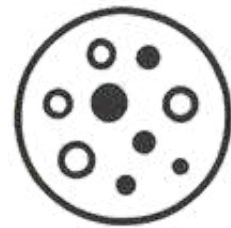
PHARMACEUTICALS



DYES



PESTICIDES



MICROPLASTICS



HEAVY METALS



HORMONES



PERSONAL CARE PRODUCTS



NANOMATERIALS



MICROORGANS



MORE

Environment International
Volume 155, October 2021, 106702

Pharmaceuticals and other urban contaminants threaten Amazonian freshwater ecosystems

Andreu Rico ^{a, b, *}, Rhaul de Oliveira ^c, Gabriel Silva de Souza Nunes ^d, Cristiana Rizzi ^e, Sara Villa ^e, Isabel López-Heras ^a, Marco Vighi ^a, Andrea Viviana Wachman ^f

Show more

Research Article

Using native fish in eco-genotoxic assessment of heavy metal contamination pollution arising from nearby large Brazilian rivers

Carine de Mendonça Francisco, Luiz Alfredo Pavanin

Pages 74-85 | Published online: 10 Jun 2023

Cite this article: <https://doi.org/10.1080/10704945.2023.2233333>



Environment International
Volume 165, July 2022, 107321

Full length article

Widespread pesticide contamination of drinking water and impact on cancer risk in Brazil

Carolina Panis ^{a, b, *}, Luciano Zanetti Pessoa Candiotti ^c, Shaiane Carla Gaboardi ^d, Susie Gurzenda ^e, Jurandir Cruz ^{b, f}, Marcia Castro ^e, Bernardo Lemos ^{b, *}



Science of The Total Environment
Volume 946, 10 October 2024, 174150



Microplastic pollution in the Amazon Basin: Current scenario, advances and perspectives

Jackiely dos Santos Silva ^a, Mirla Janaina Augusta Cidade ^a, Francisco dos Santos Panero ^{a, b}, Leila Braga Ribeiro ^a, Franciele Oliveira Campos da Rocha ^{a, b, *}

JOURNAL ARTICLE

COVID-19 Therapies in Brazil: Should We Be Concerned with the Impacts on Aquatic Wildlife?

Davi Felipe Farias ^{*}, Terezinha Souza, Juliana Alves Costa Ribeiro Souza, Leonardo Rogério Vieira, Marta Silva Muniz, Rafael Xavier Martins, Íris Flávia Sousa Gonçalves, Eduardo Afonso Silva Pereira, Maria Eduarda Souza Maia, Marília Guia Flor Silva

Environmental Toxicology and Chemistry, Volume 39, Issue 12, 1 December 2020, Pages 2348–2350, <https://doi.org/10.1002/etc.4888>

Published: 02 October 2020 Article history



WATER AT NANOSCALE

Motivation

Contaminantes of Emerging Concern



Journal of Environmental Management
Volume 371, December 2024, 122995

Research article
Tackling water contamination by oncologic drugs: Supported ionic liquids as sustainable adsorbents for cyclophosphamide removal

Rafael Francisco ^{a 1}, Bruna Monteiro ^{a b 1}, Maria J. Santos ^a, Francisca A. e Silva ^a, Catia Venancio ^b, Marcia C. Neves ^a, Isabel Lopes ^b, Ana C.A. Sousa ^c, Mara G. Freire ^a



Environment International

Volume 164, June 2022, 107281

Full length article

Drugs of abuse in tap water from eight European countries: Determination by use of supramolecular solvents and tentative evaluation of risks to human health

Luis Muñiz-Bustamante, Noelia Caballero-Casero, Soledad Rubio



Chemosphere
Volume 356, May 2024, 141699

Emerging organic contaminants in drinking water systems: Human intake, emerging health risks, and future research directions

Jerikias Marumure ^{a b}, Tinoziva T. Simbanegavi ^c, Zakio Makuvara ^{a b}, Rangarirayi Karidzagundi ^d, Richwell Alufasi ^e, Marvelous Goredema ^e, Claudious Gufe ^f, Nhamo Chaukura ^g, Dariusz Halabowski ^h, Willis Gwenzi ^{i j k}

Home > Environmental Science and Pollution Research > Article

Occurrence of pharmaceutical residues in drinking water: a systematic review

Emerging Chemical Pollution of the Planet | Published: 06 August 2024

Volume 32, pages 10436–10463, (2025) [Cite this article](#)

Review article

Emerging contaminants in surface waters and their relevance for the production of drinking water in Europe

Corine J. Houtman

Pages 271-295 | Received 21 Apr 2010, Accepted 26 Jul 2010, Published online: 24 Sep 2010

[Cite this article](#) <https://doi.org/10.1080/1943815X.2010.511648>

WATER AT NANOSCALE

Motivation

Contaminantes of Emerging Concern



19.10.2021 in News 0, 1330

Mercury, tramadol, industrial chemicals and even caffeine: scientists presented the results of the analysis of the pollutants concentrations in the flora and fauna of Antarctica





EMERGING CONTAMINANTS



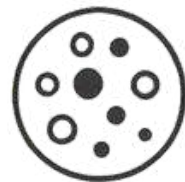
PHARMACEUTICALS



DYES



PESTICIDES



MICROPLASTICS



HEAVY METALS



HORMONES

PERSONAL CARE
PRODUCTS

NANOMATERIALS



MICROORGANS



MORE

Segurança hídrica

Contaminantes emergentes agravam crise hídrica nos países em desenvolvimento, aponta dossiê

28 de abril de 2025

Além da escassez e da distribuição desigual da água, a qualidade está sendo fortemente afetada por pesticidas de uso agrícola, resíduos industriais e descarte de medicamentos e produtos de higiene

José Tadeu Arantes | Agência FAPESP – Com o crescimento da população, da urbanização e da atividade agroindustrial, o uso global de água doce deverá aumentar 55% até 2050. A projeção dos estudiosos é que essa escalada da demanda venha a impactar fortemente um cenário já caracterizado pela escassez e distribuição desigual dos recursos hídricos, pela privatização de um bem essencial que deveria ser de domínio público e pela deterioração da qualidade da água, especialmente nos países em desenvolvimento.



Entre os poluentes emergentes estão pesticidas de uso agrícola, aditivos de combustíveis, materiais plastificantes ou antiaderentes, medicamentos, produtos de higiene e cosméticos (foto: Freepik)

Além dos contaminantes, o pesquisador chama atenção para um problema estrutural mais amplo: a desigualdade no acesso à água e os efeitos já observáveis das mudanças climáticas. "As grandes enchentes, como vimos recentemente no Rio Grande do Sul, comprometem toda a estrutura de captação e distribuição de água potável. Por outro lado, há regiões que estão enfrentando secas severas. Entre 2002 e 2021, as secas afetaram mais de 1,4 bilhão de pessoas", diz.



Science of The Total Environment
Volume 836, 25 August 2022, 155605



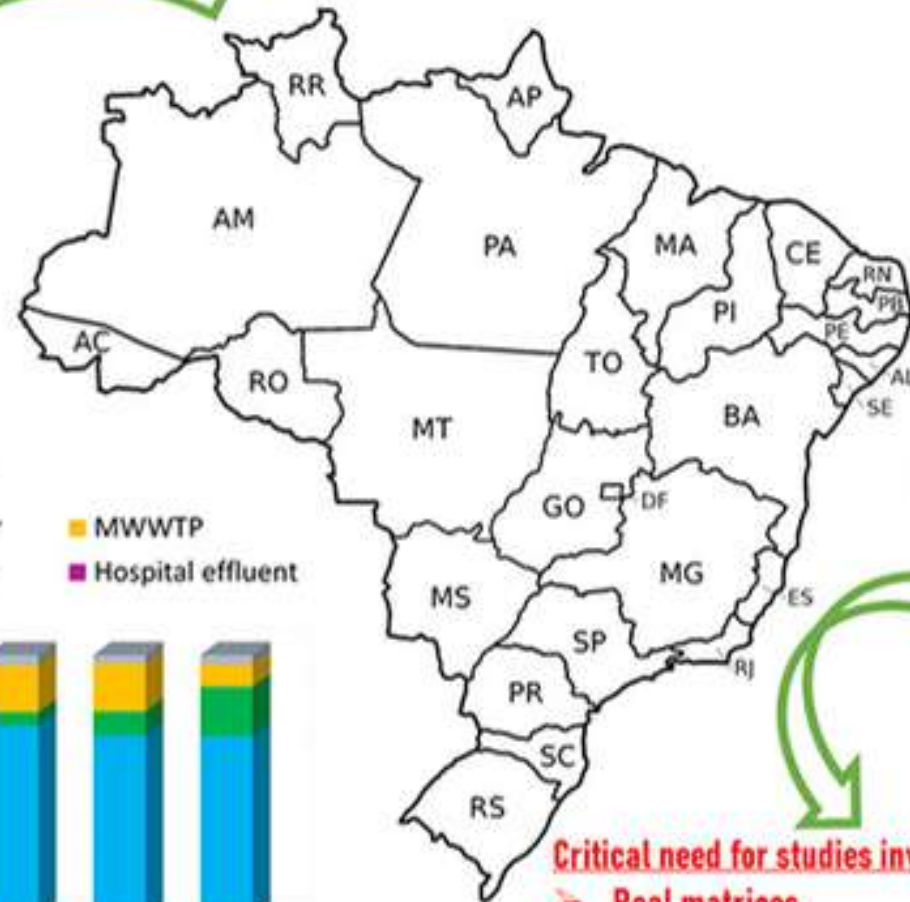
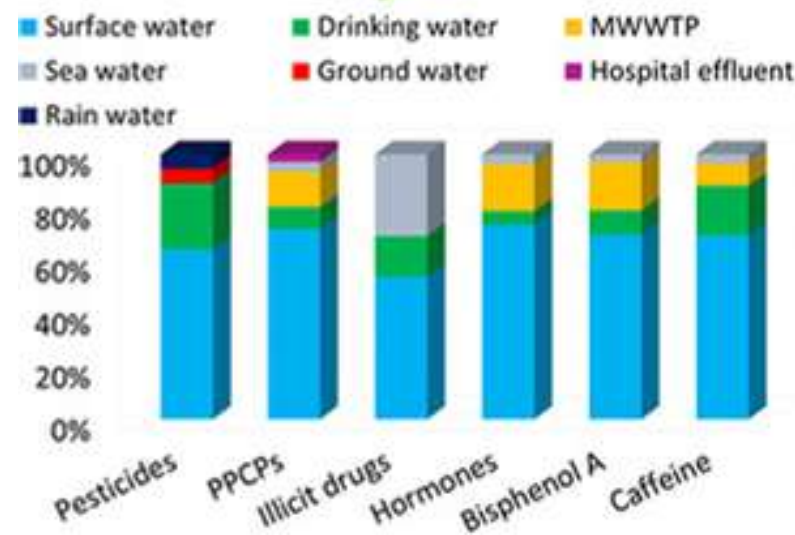
Review

A review toward contaminants of emerging concern in Brazil: Occurrence, impact and their degradation by advanced oxidation process in aquatic matrices

Eduardo O. Marson^a, Cleisano E.S. Paniagua^a, Oswaldo Gomes Júnior^a, Bárbara R. Gonçalves^a, Valdislaine M. Silva^a, Ivo A. Ricardo^{a,b}, Maria Clara V. M. Starling^c, Camila C. Amorim^c, Alam G. Trovó^a

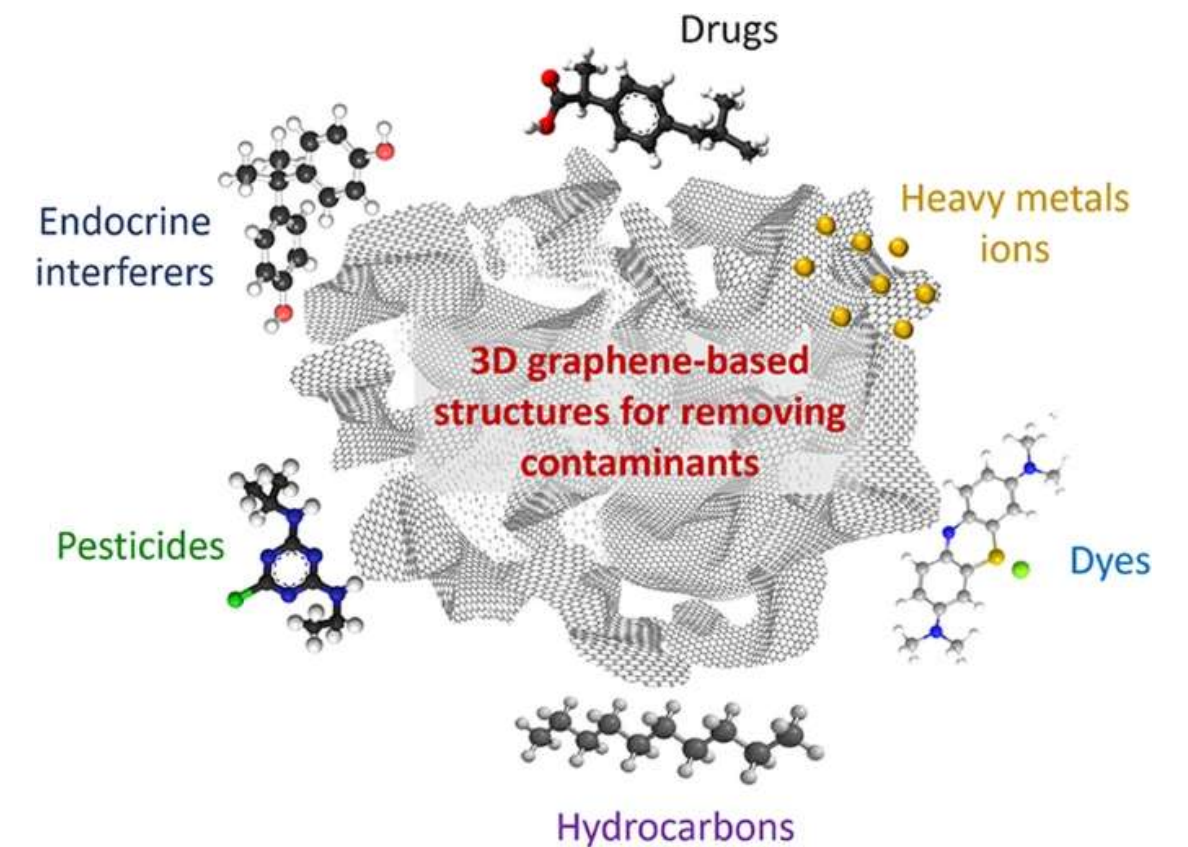
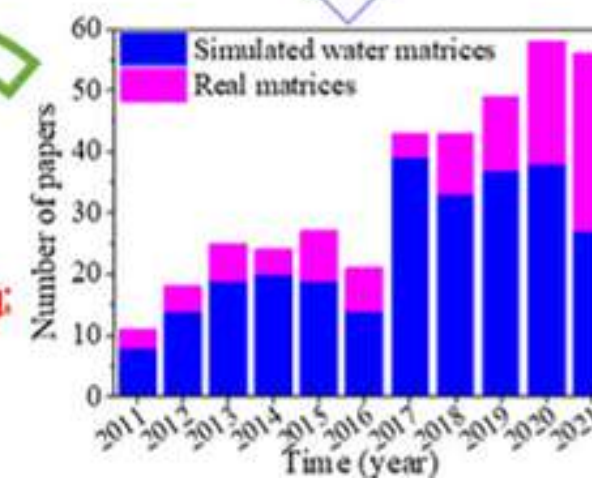
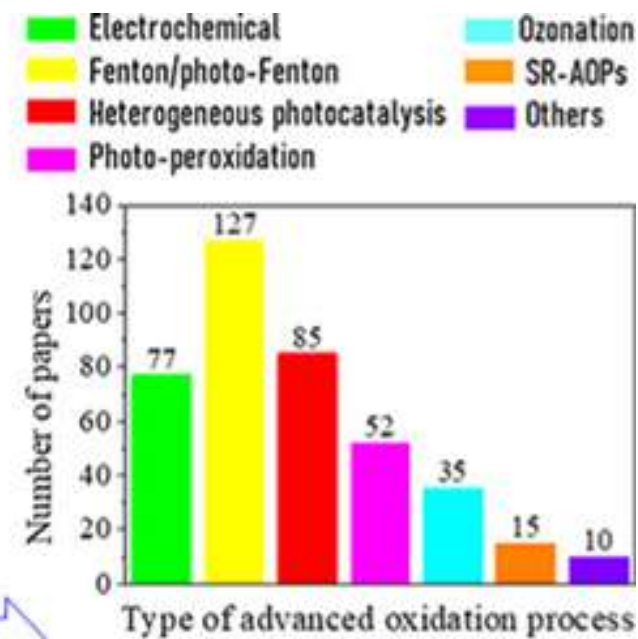


- 87 pharmaceuticals and personal care products
- 58 pesticides
- 8 hormones
- 2 illicit drugs
- Caffeine
- Bisphenol A



Critical need for studies involving:

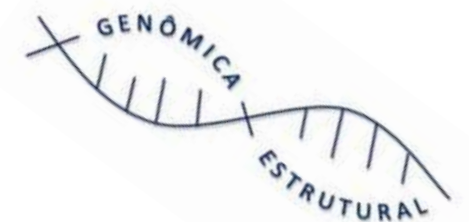
- Real matrices
- Toxicity assessment
- Evaluation of water reuse



CECs



CECs at our door



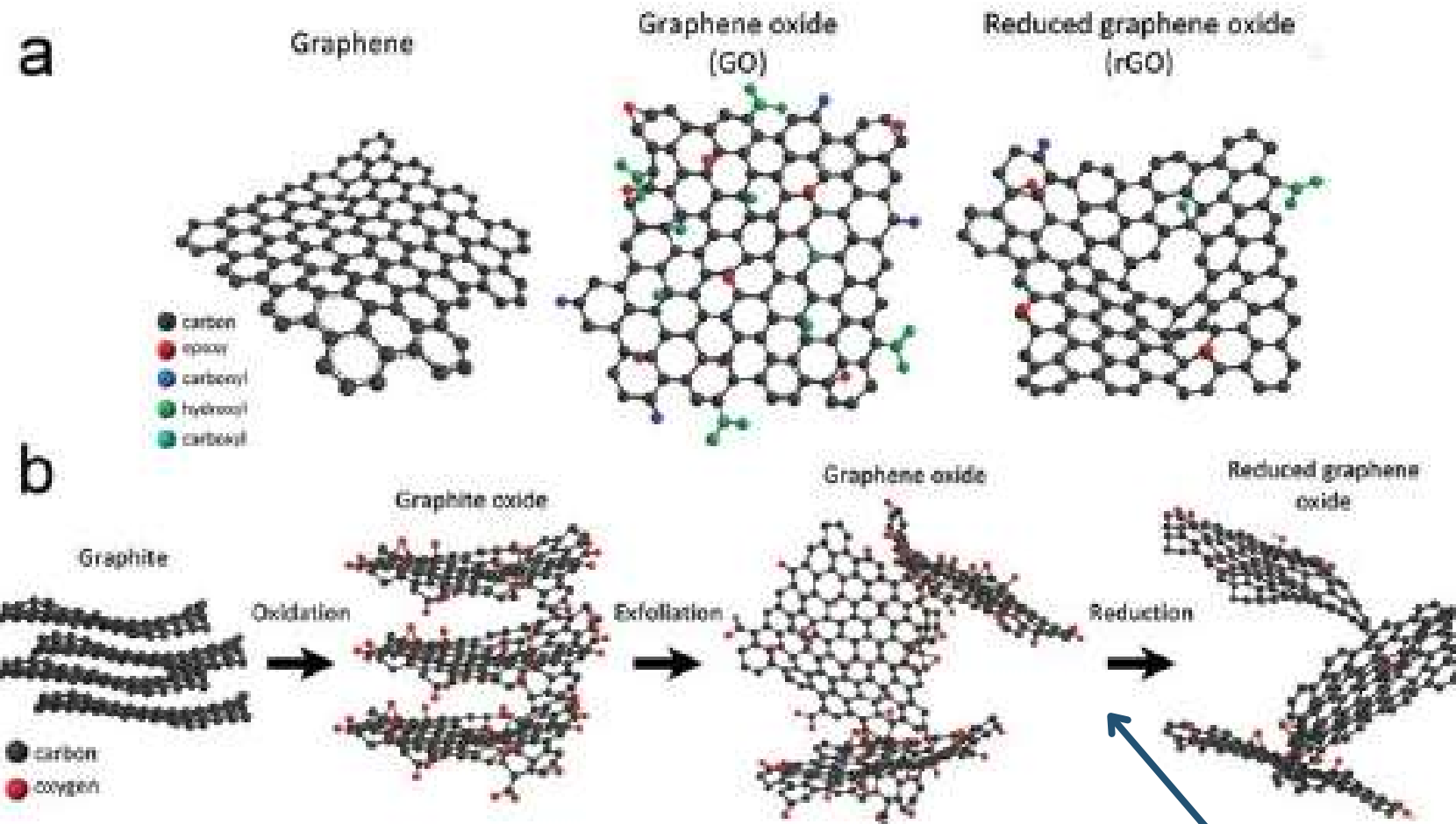
**VINICIUS CAMPOS
& TONY SILVEIRA**
BIOTEC/UFPEL

WATER AT NANOSCALE



graphene oxide sponges

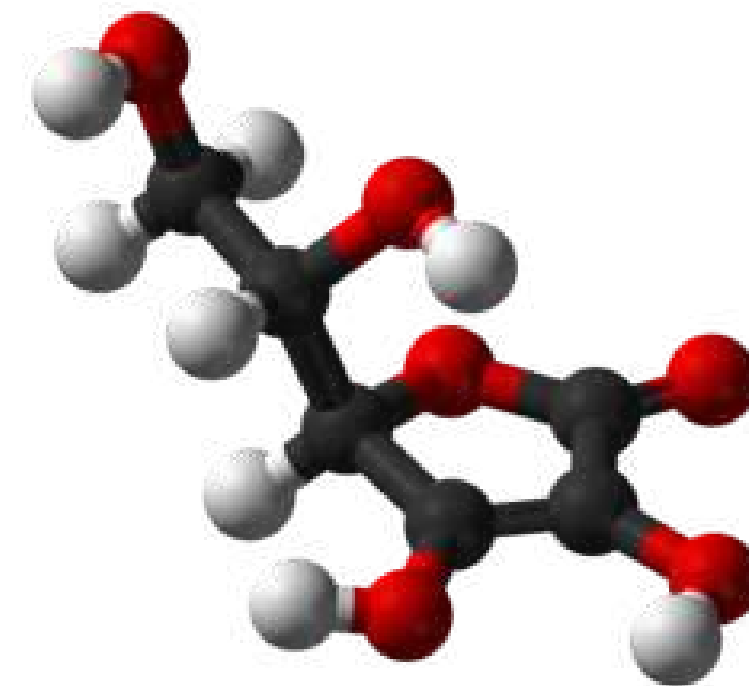
creating the nanomaterial



MAYARA B. LEÃO
GQMATE (UNIPAMPA)

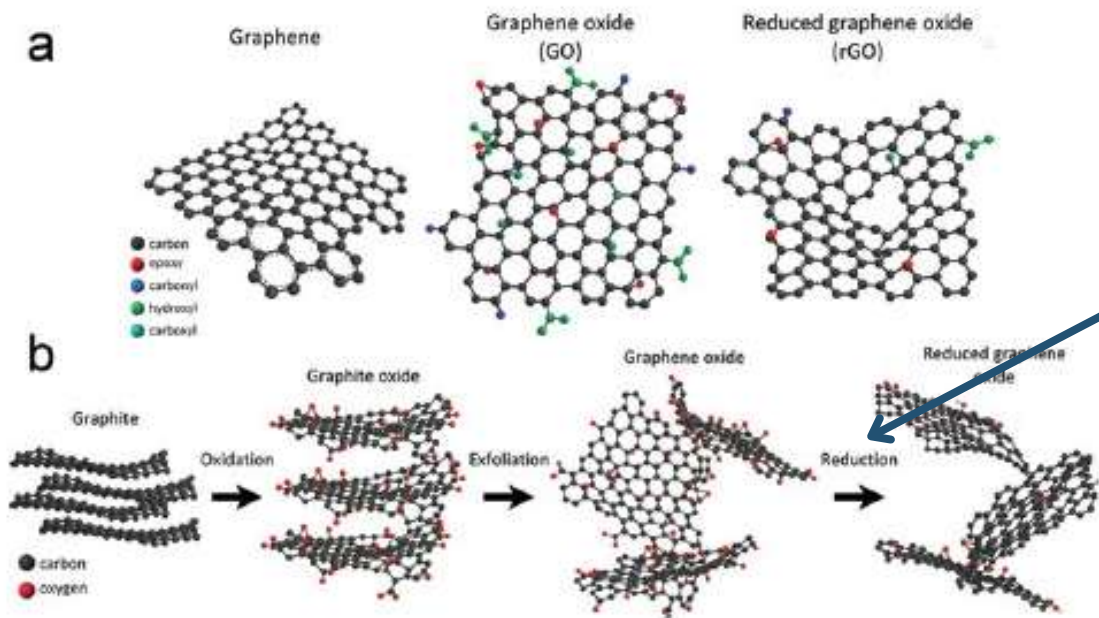


CAROLINA F. M. JAURIS
GRUPO DE QUÍMICA DE MATERIAIS (UFSM)



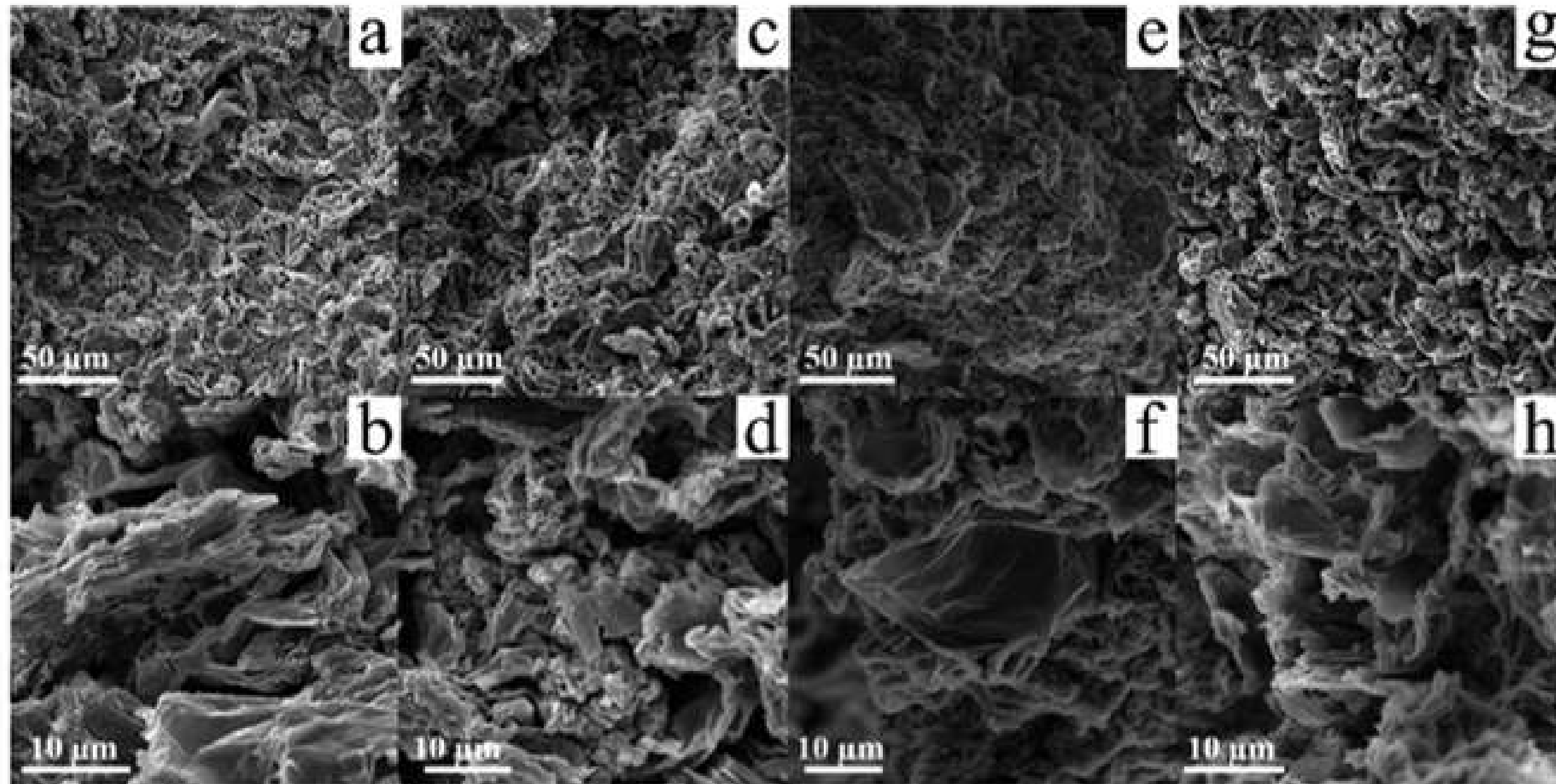
graphene sponges

eco, cheap, fast!



Temos a grata satisfação de informar que o INPI emitiu um novo parecer sobre o depósito BR 10 2020 010054 8 “*Processo de obtenção de estruturas tridimensionais baseadas em grafeno*”, através do documento 1735801, que **defer**e pedido como patente de invenção.

Informamos que estamos providenciando a emissão e liquidação da GRU correspondente à carta patente.



Scanning electron microscopy of materials (a and b) 3D-rGO0, (c and d) 3D-rGO5, (e and f) 3D-rGO10 and (g and h) 3D-rGO25.



MSDE

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Cite this: DOI: 10.1039/d2me00268j

Combining multi-scale simulations and experiments to unveil the adsorption of methylene blue in graphene tridimensional-based materials†Mayara B. Leão,^a Laura F. O. Vendrame,^b Solange B. Fagan,^b Ivana Zanella,^b Iuri M. Jauris,^c José R. Bordin^d and Carolina F. de Matos^{a*}**Table 6** Comparison of the results obtained with works available in the literature

Material	Specific surface area (m ² g ⁻¹)	Q _{max} (mg g ⁻¹)	Contact time (h)	References
3D-rGO0	172.274	705.81	5	This work
3D-rGO5	163.198	1034.70	5	This work
3D-rGO10	68.980	317.65	5	This work
3D-rGO25	62.807	227.57	5	This work
Tannic acid functionalized graphene hydrogel	196.57	714.3	12	Tang <i>et al.</i> , 2018 (ref. 14)
rGO hydrogel/decylamine	47.8	482	24	Zheng <i>et al.</i> , 2021 (ref. 47)
Three-dimensional graphene aerogels	1099.43	221.77	4	Trinh <i>et al.</i> , 2021 (ref. 46)
rGO sheets consolidated by cross-linked sodium alginate	23.59	192.3	24	Ma <i>et al.</i> , 2014 (ref. 15)

Dye



Methylene Blue



WATER AT NANOSCALE

MSDE

PAPER



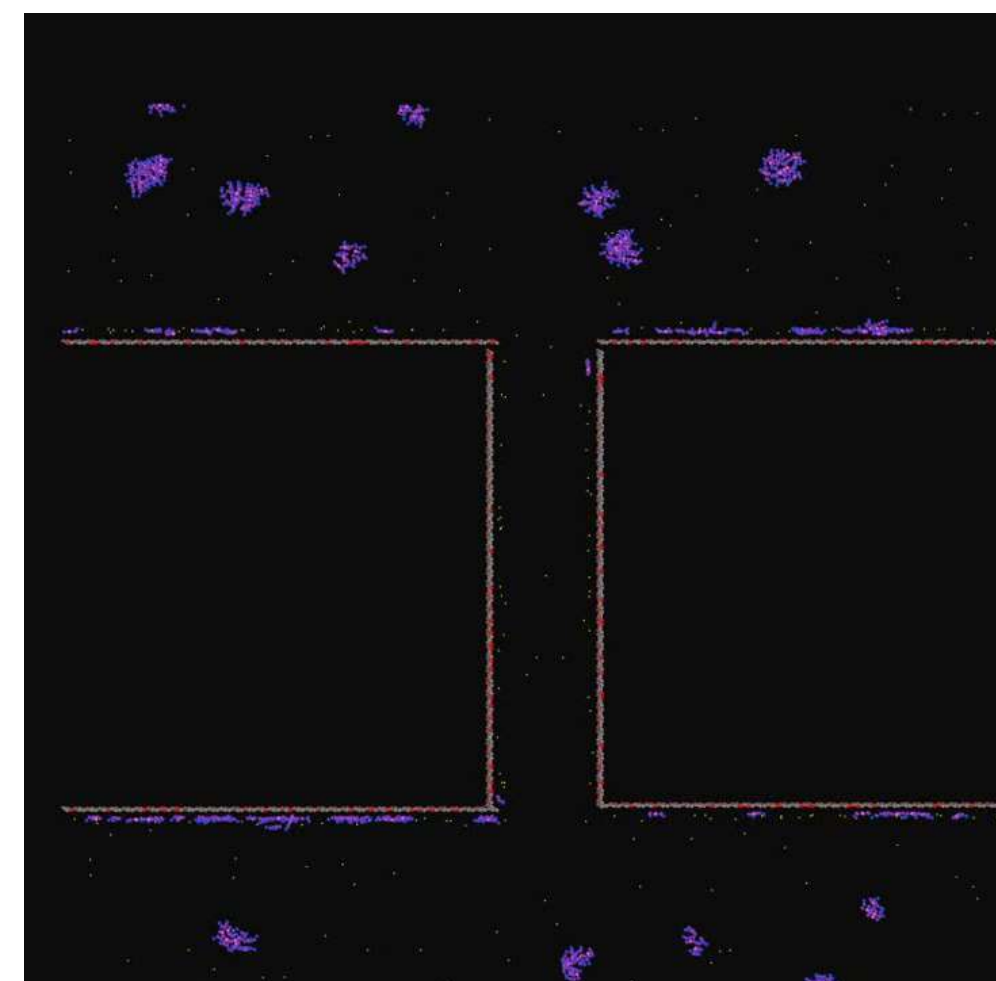
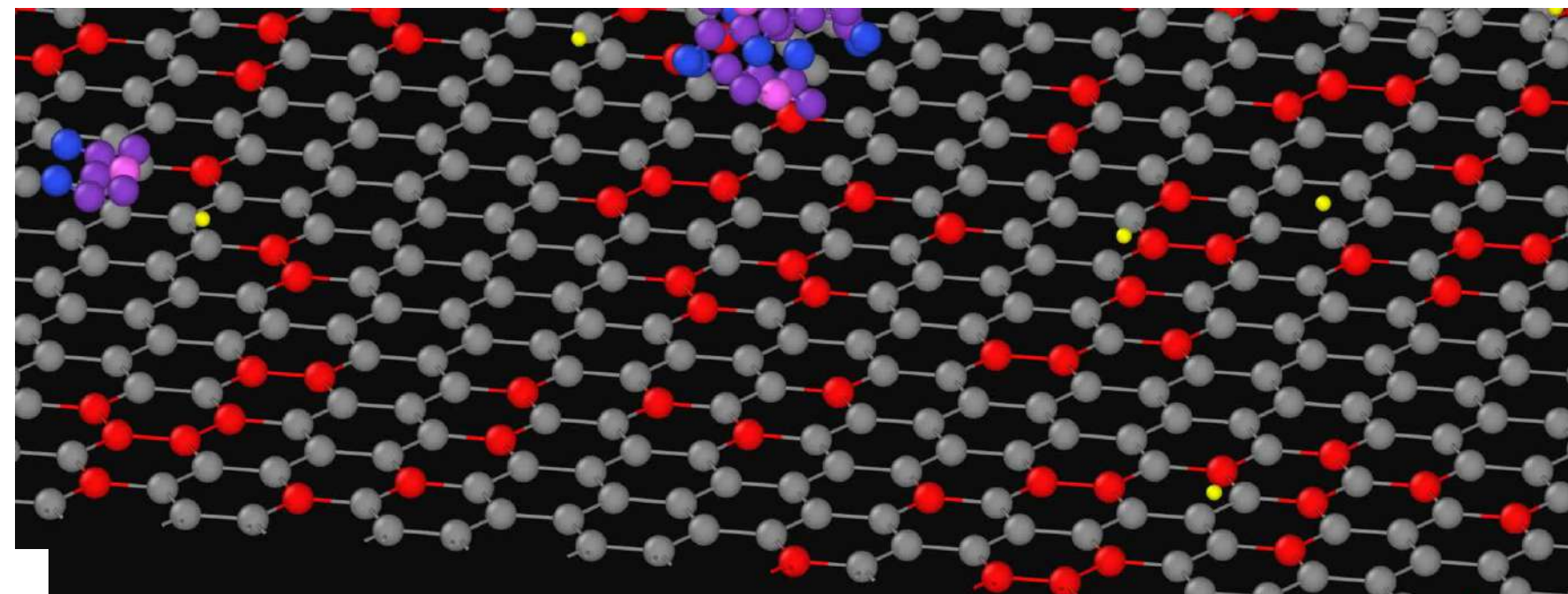
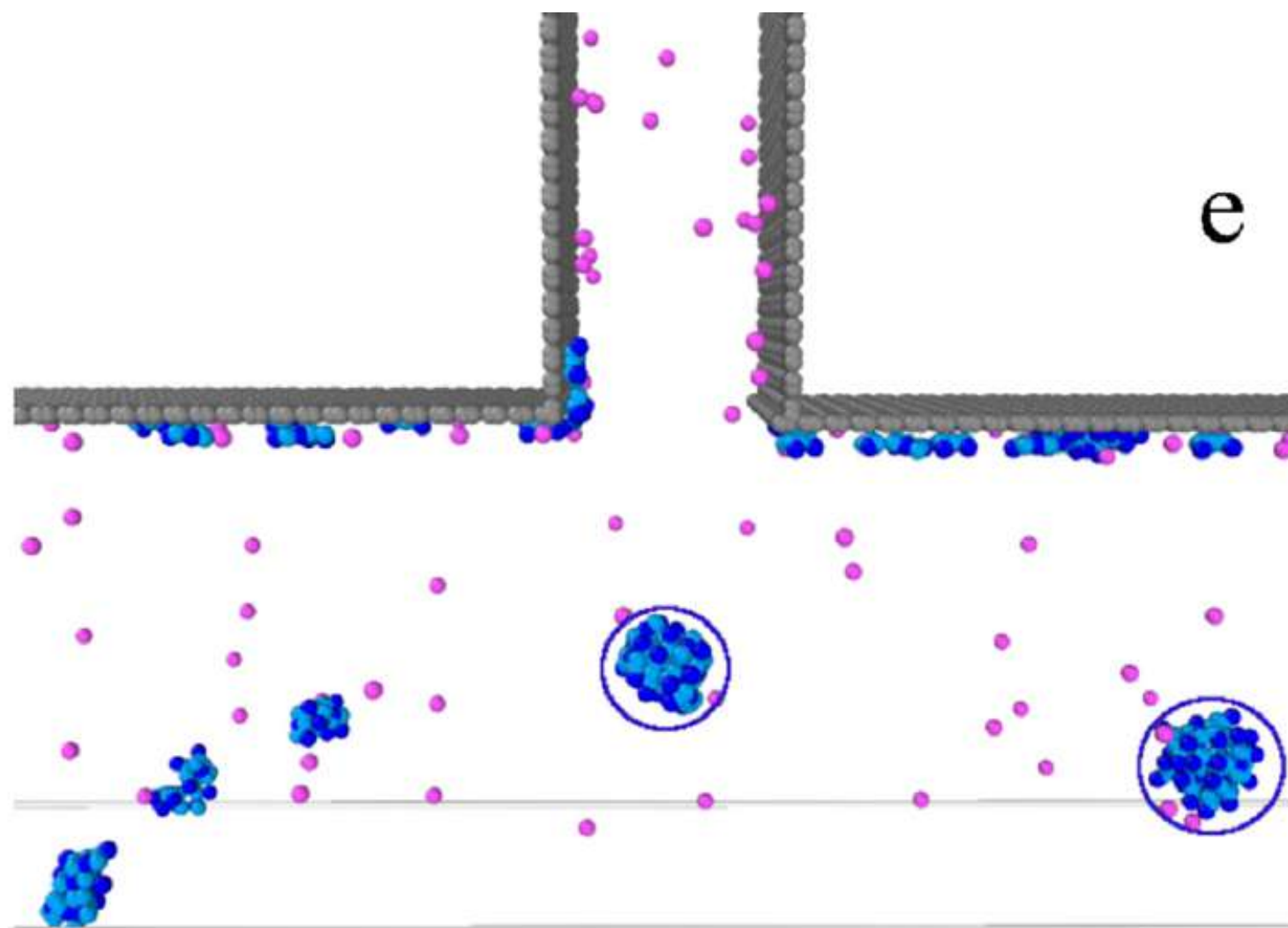
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Combining multi-scale simulations and experiments to unveil the adsorption of methylene blue in graphene tridimensional-based materials†

Mayara B. Leão,^a Laura F. O. Vendrame,^b Solange B. Fagan,^b Ivana Zanella,^b Iuri M. Jauris,^c José R. Bordin^d and Carolina F. de Matos^{*a}



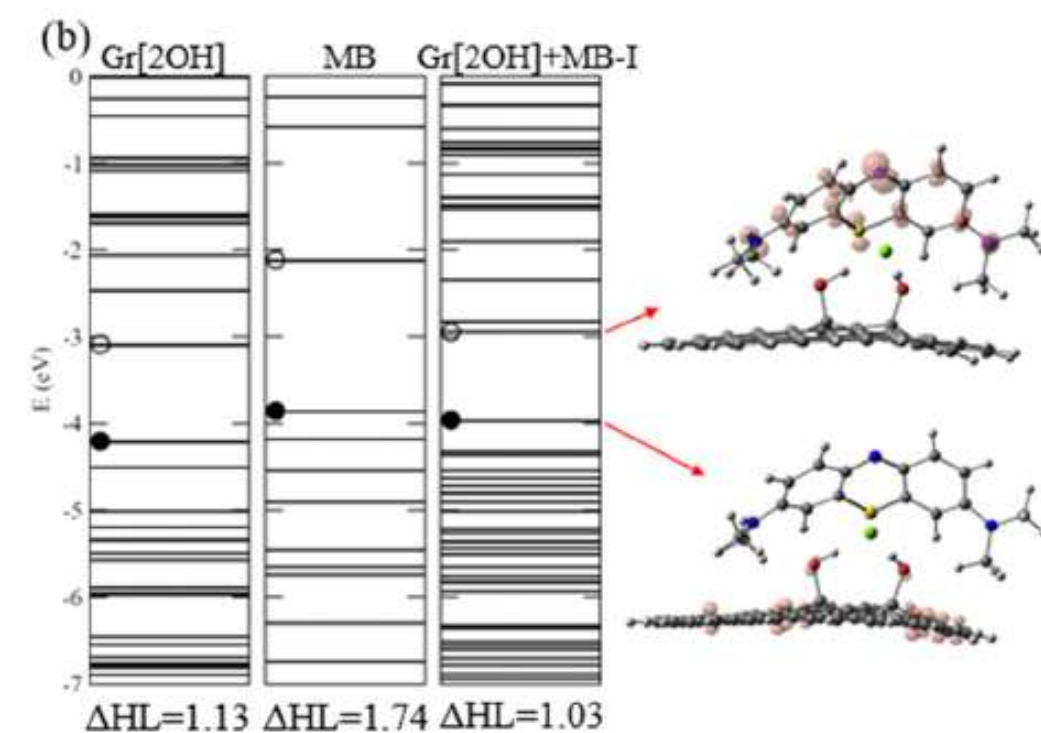
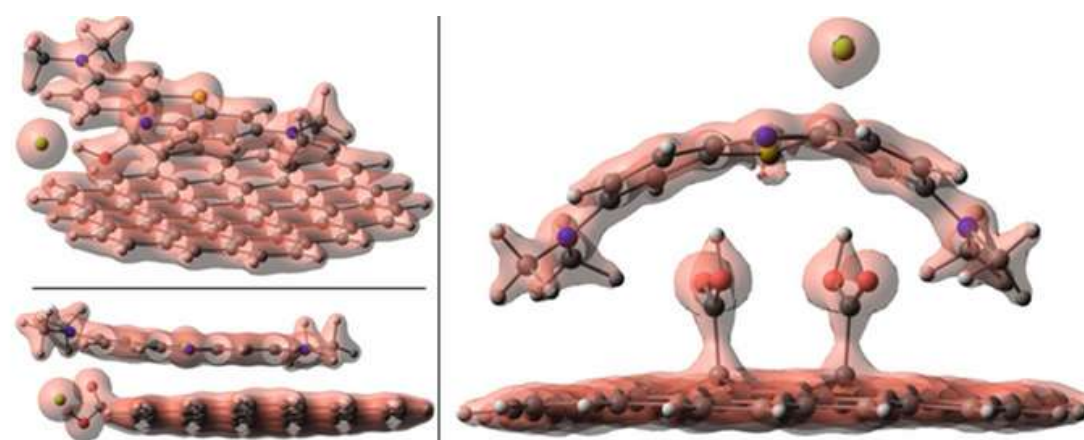
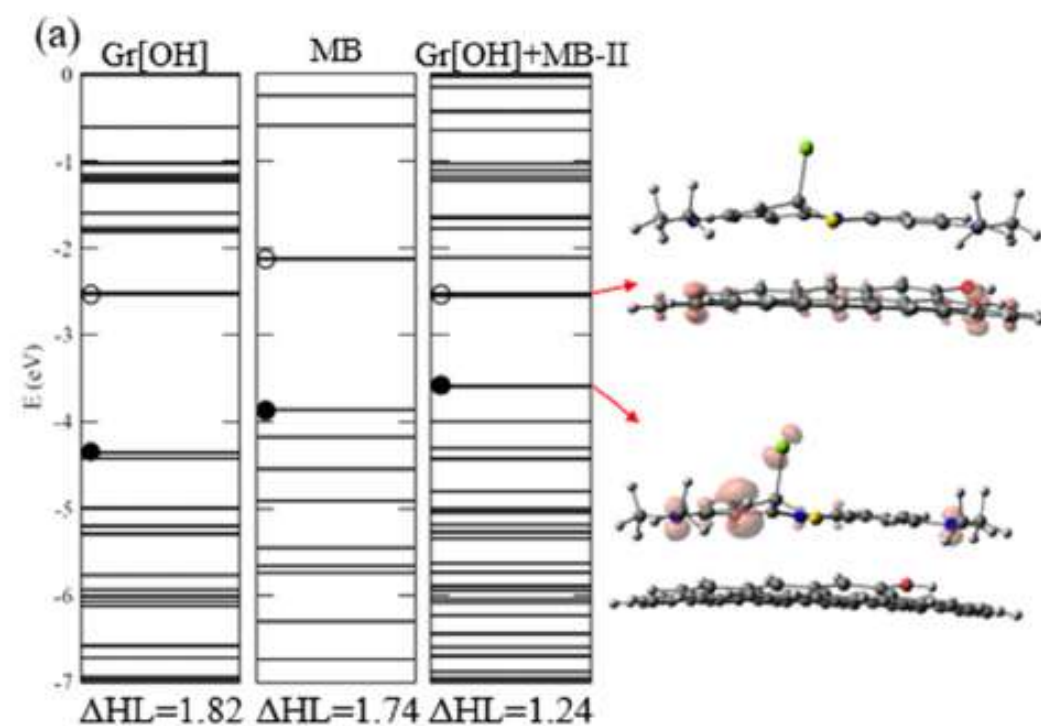
Dye



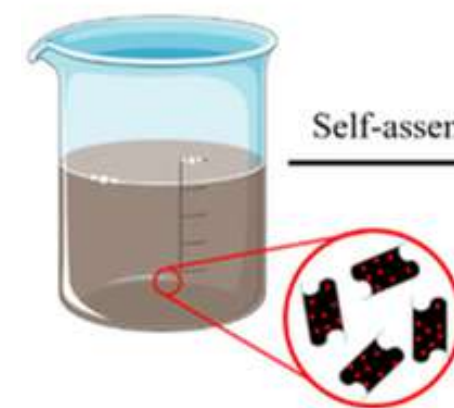
Methylene Blue



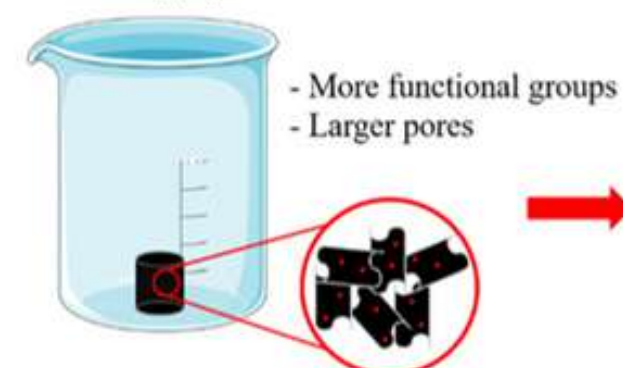
**SOLANGE FAGAN
LASIMON -
UNIVERSIDADE
FRANCISCANA (UFN) -
SANTA MARIA**



Graphene Oxide

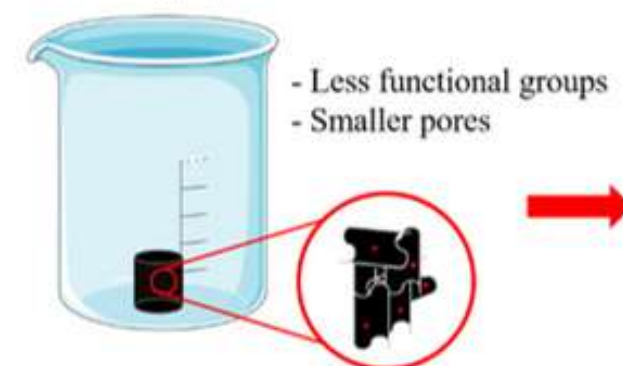


Less amount of
reducing agent



- High
Adsorption
- Higher
Interaction
Energy

Higher amount of
reducing agent



Clusters
Low
adsorption

Graphene sheet
Oxygenated functional group

WATER AT NANOSCALE

Pesticides



Glyphosate



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Research Article

Quantum Simulations and Experimental Insights into Glyphosate Adsorption Using Graphene-Based Nanomaterials

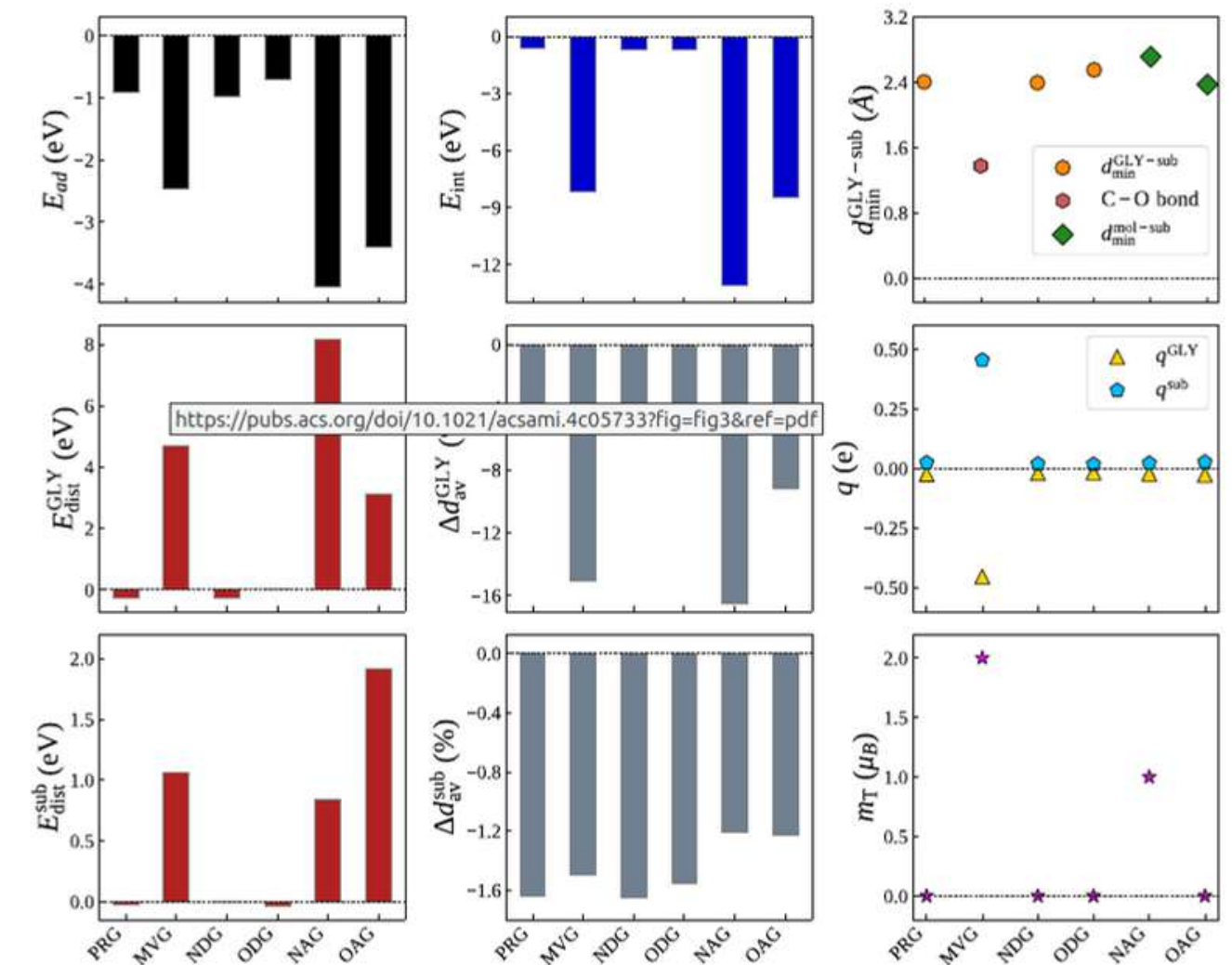
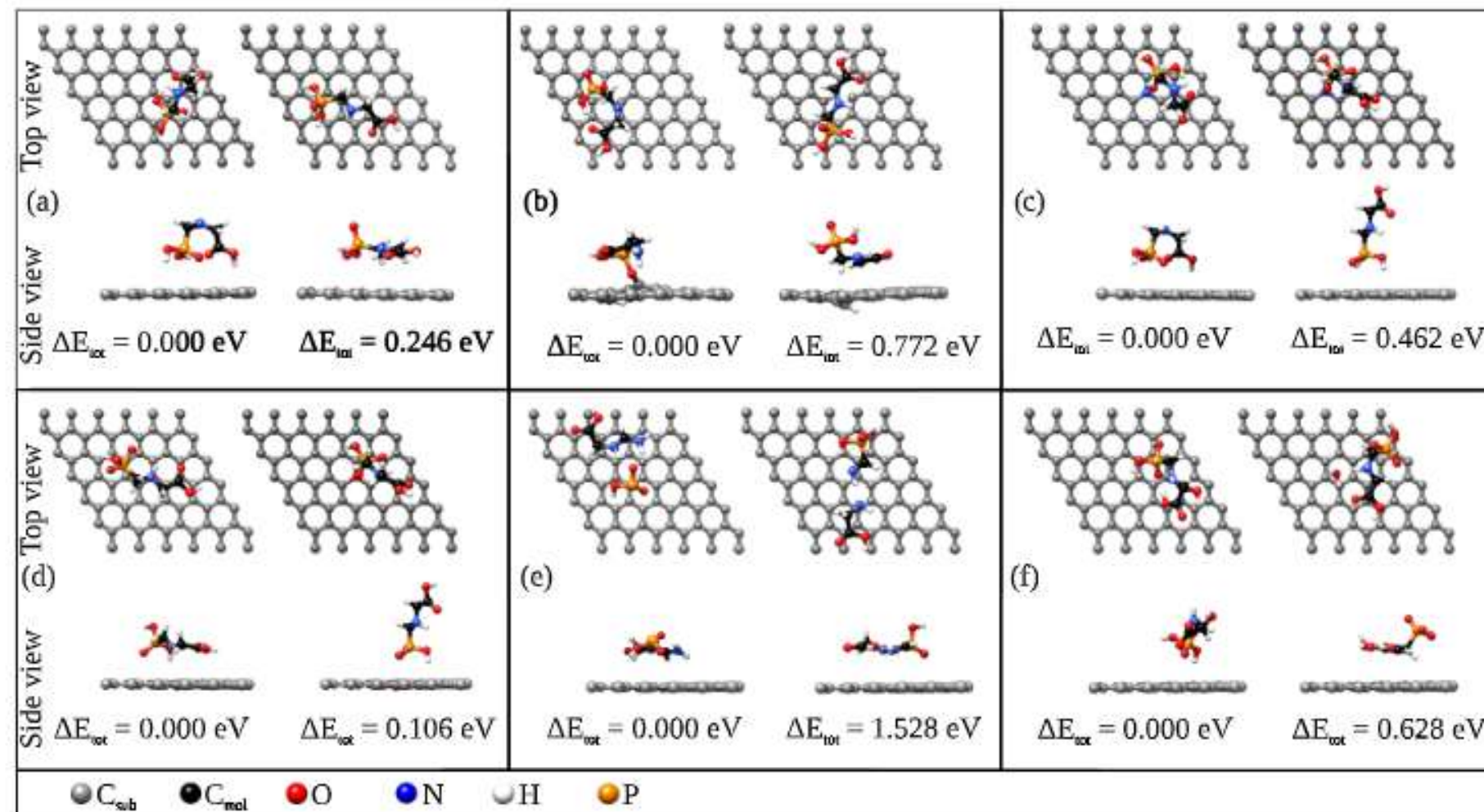
Wanderson S. Araújo, Celso Ricardo Caldeira Rêgo,* Diego Guedes-Sobrinho, Alexandre Cavaleiro Dias, Isadora Rodrigues do Couto, José Rafael Bordin, Carolina Ferreira de Matos, and Maurício Jeomar Piotrowski

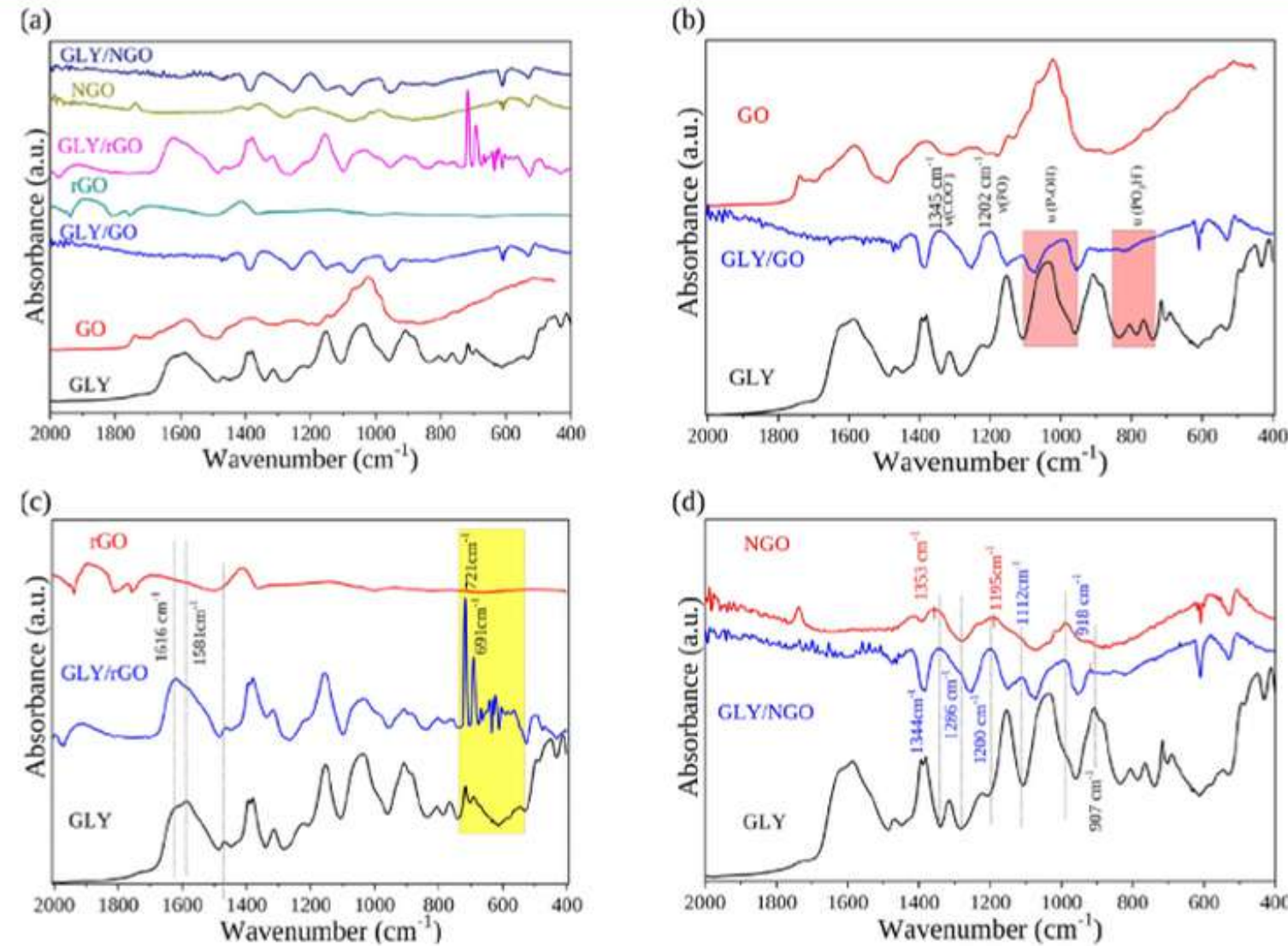


WANDERSON ARAÚJO
PHD (UFPEL)

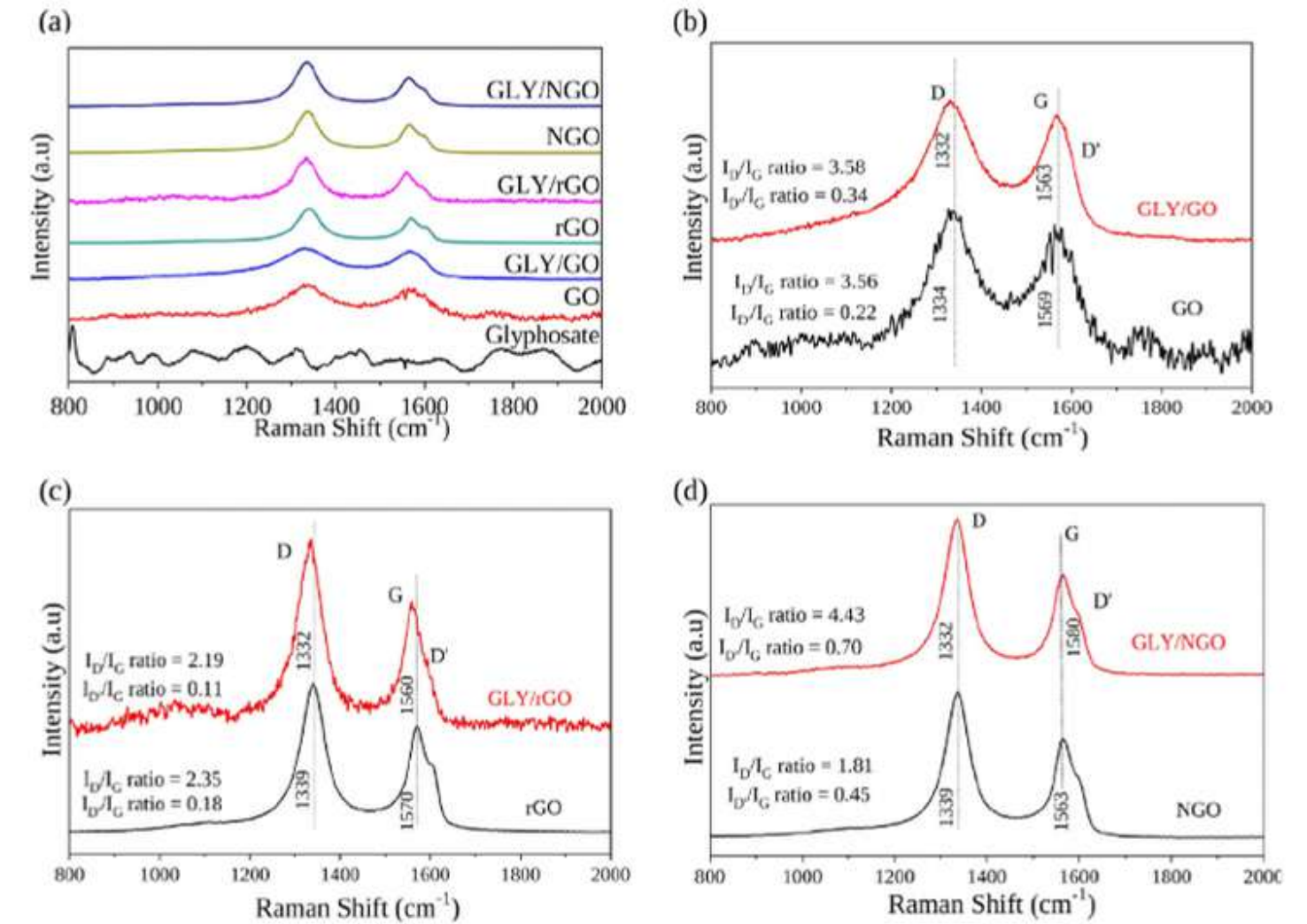


MAURICIO PIOTROWSKI
(UFPEL)





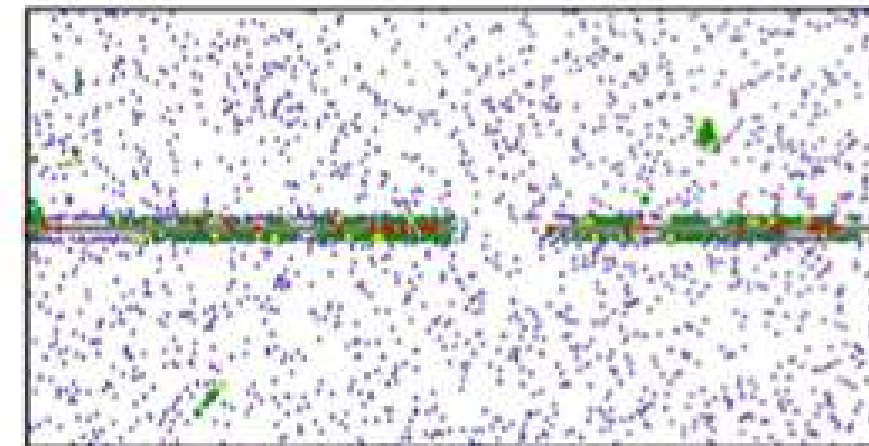
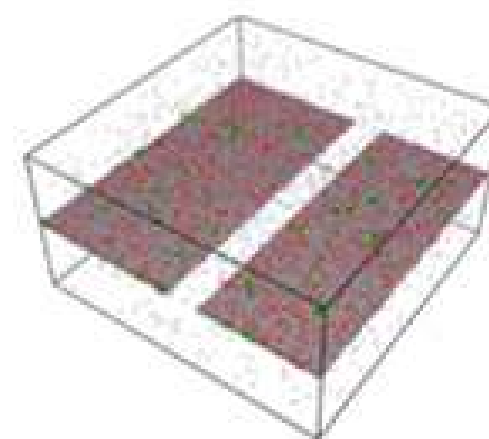
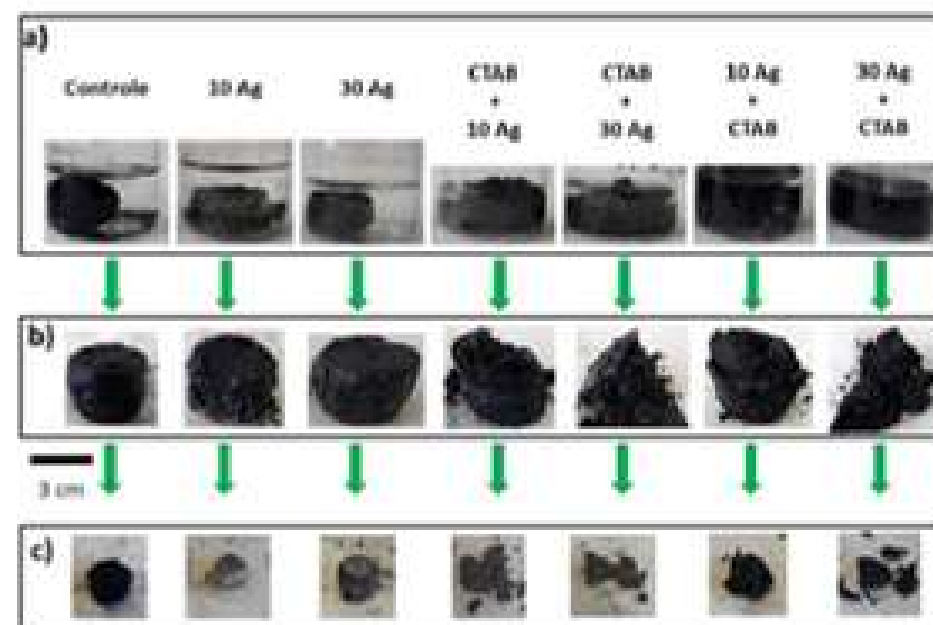
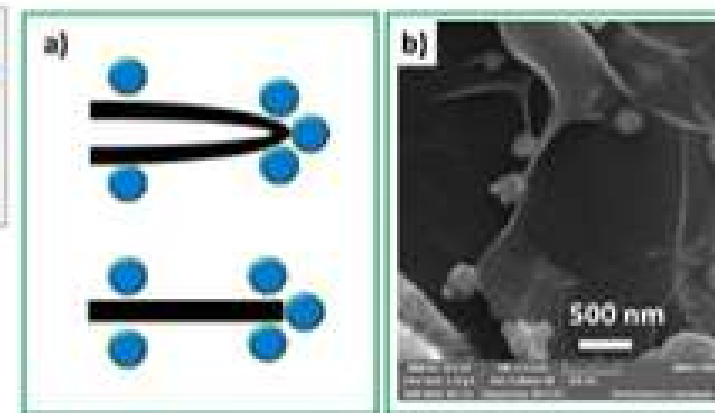
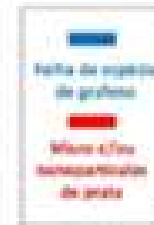
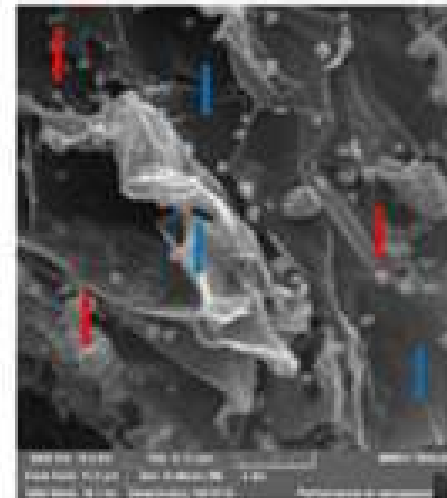
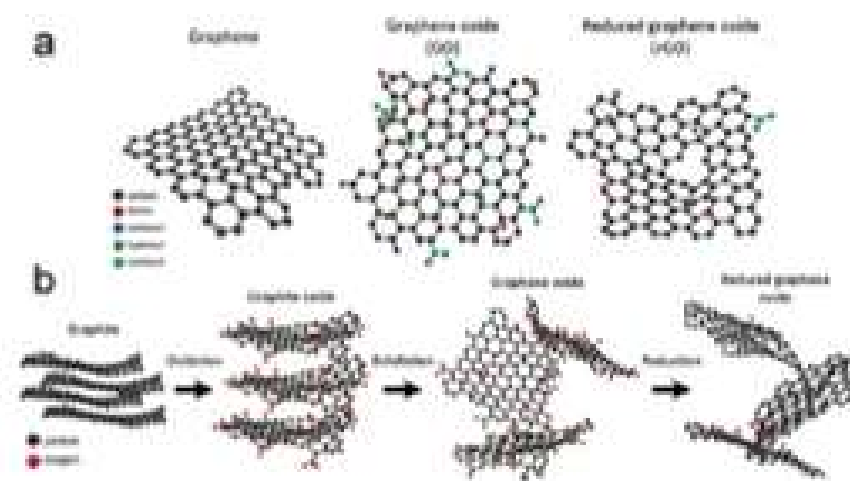
IR studies before and after GLY adsorption: (a) GLY, GO, rGO, and NGO; (b) GO; (c) rGO; and (d) NGO.



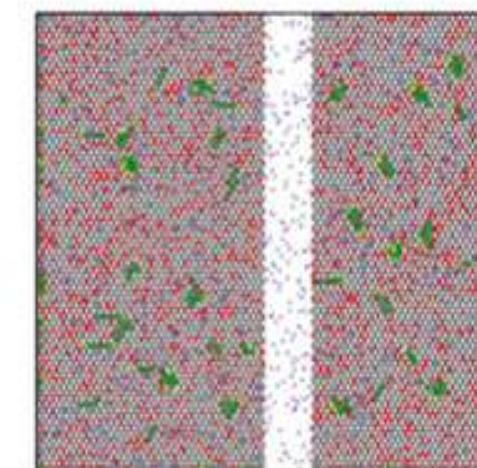
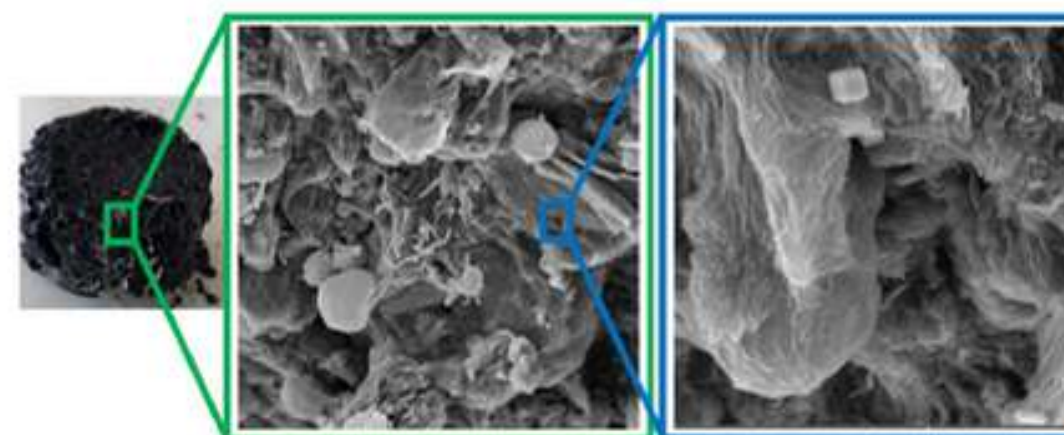
graphene sponges



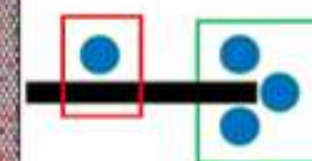
decorating with silver



Processo de Obtenção de Macroestruturas Porosas de Grafeno e Partículas de Prata. C. F. Matos, P. C. C. da Rosa and JRB. Patente: Privilégio de Inovação. Número do registro: BR10202001803, Instituição de registro: INPI - Instituto Nacional da Propriedade Industrial, Depósito PCT: 03/09/2020



Geometric effect of the edge.



PAULO DA ROSA
(UNIPAMPA)





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Article

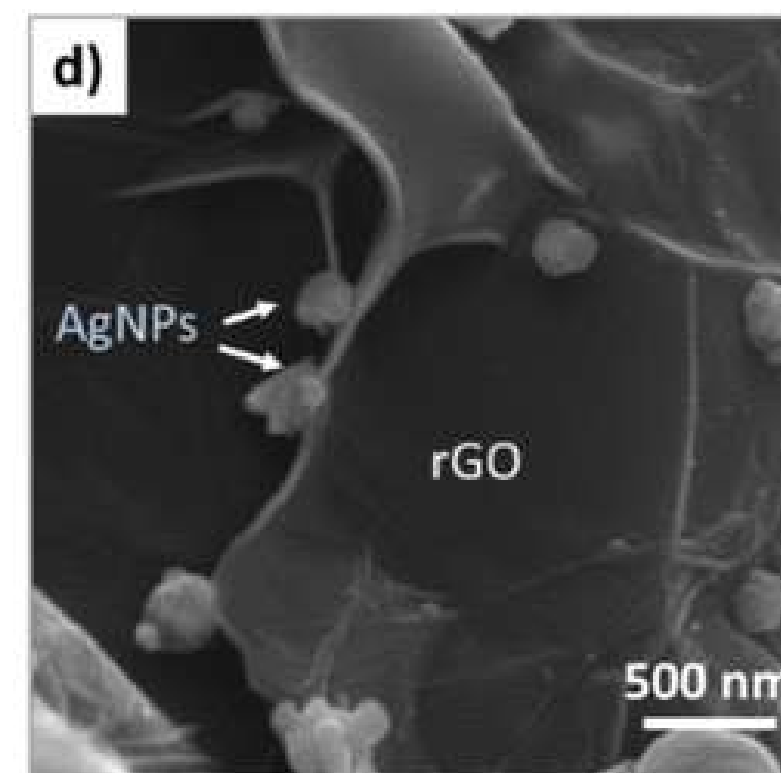
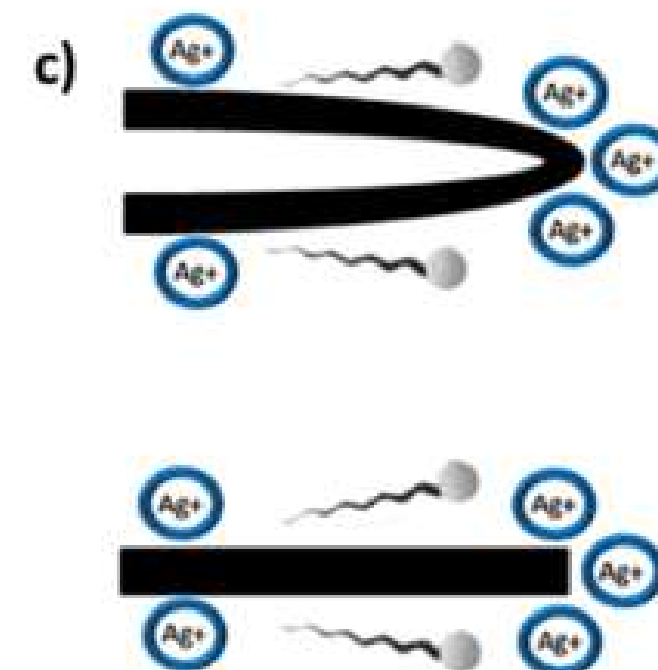
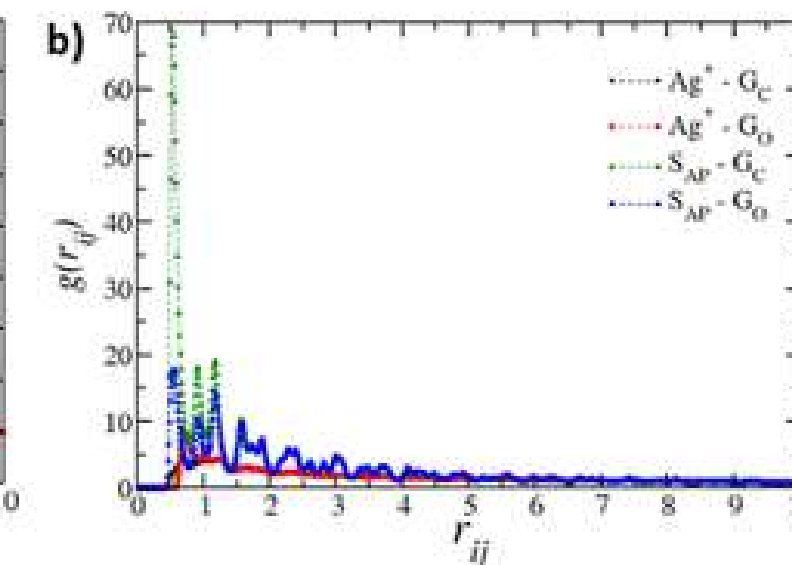
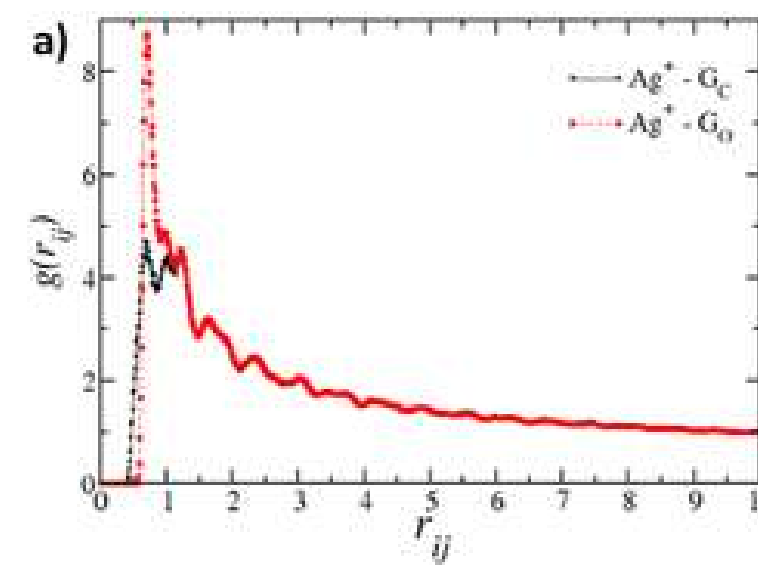
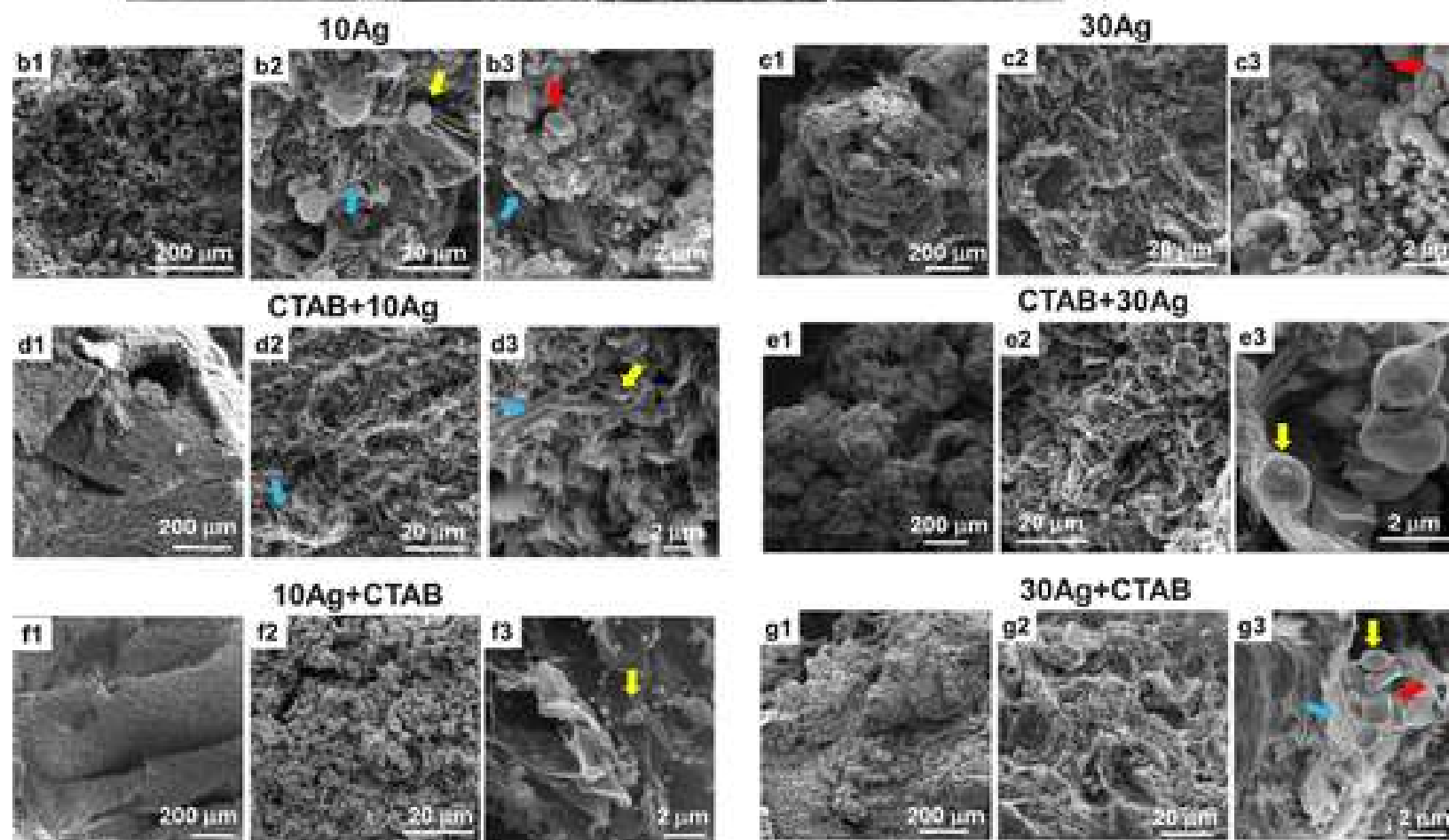
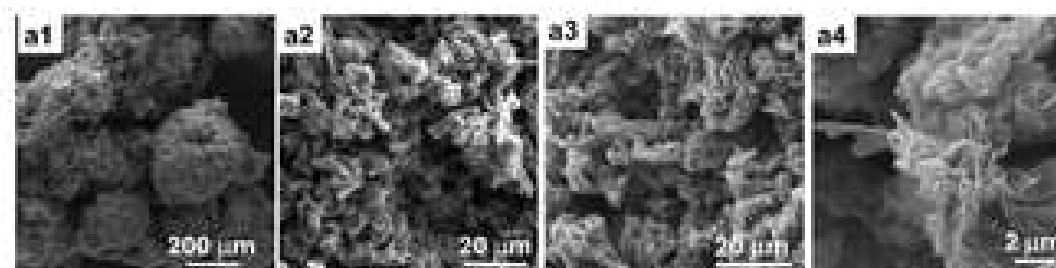
Structure-Dependent Properties of Silver-Decorated 3D-Reduced Graphene Oxide Nanocomposites: Influence of Reagent Addition Sequence and Applications in Electrochemical Sensing

Paulo Castro Cardoso da Rosa, Anna Elisa Silva, Eduardo Guilherme Cividini Neiva, José Rafael Bordin, and Carolina Ferreira de Matos Jauris*

Cite This: <https://doi.org/10.1021/acsomega.4c09382>

Read Online

Control



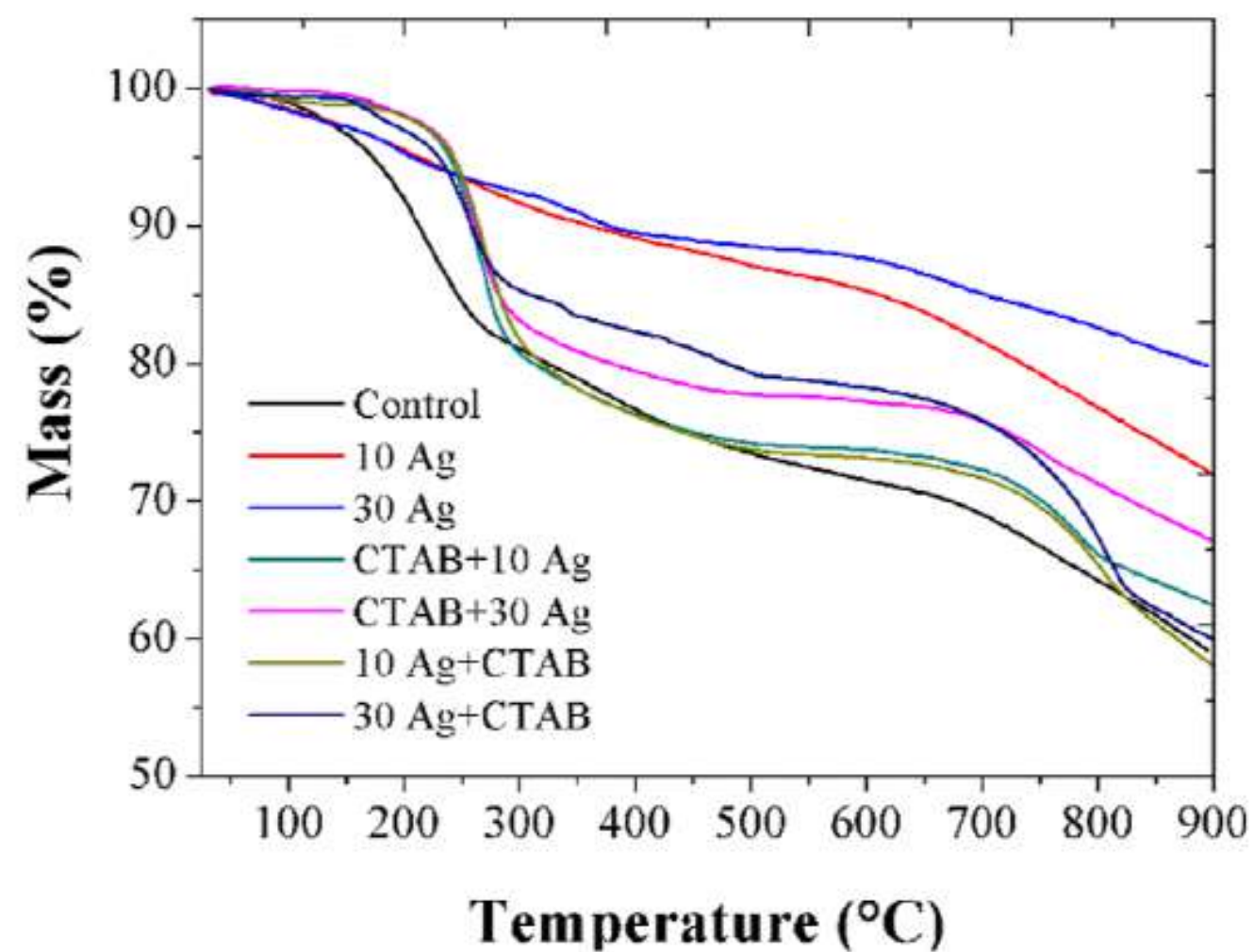


Figure 5. TGA curves of the different macrostructures collected in a nitrogen atmosphere.



EDUARDO C. NEIVA
(FURB)

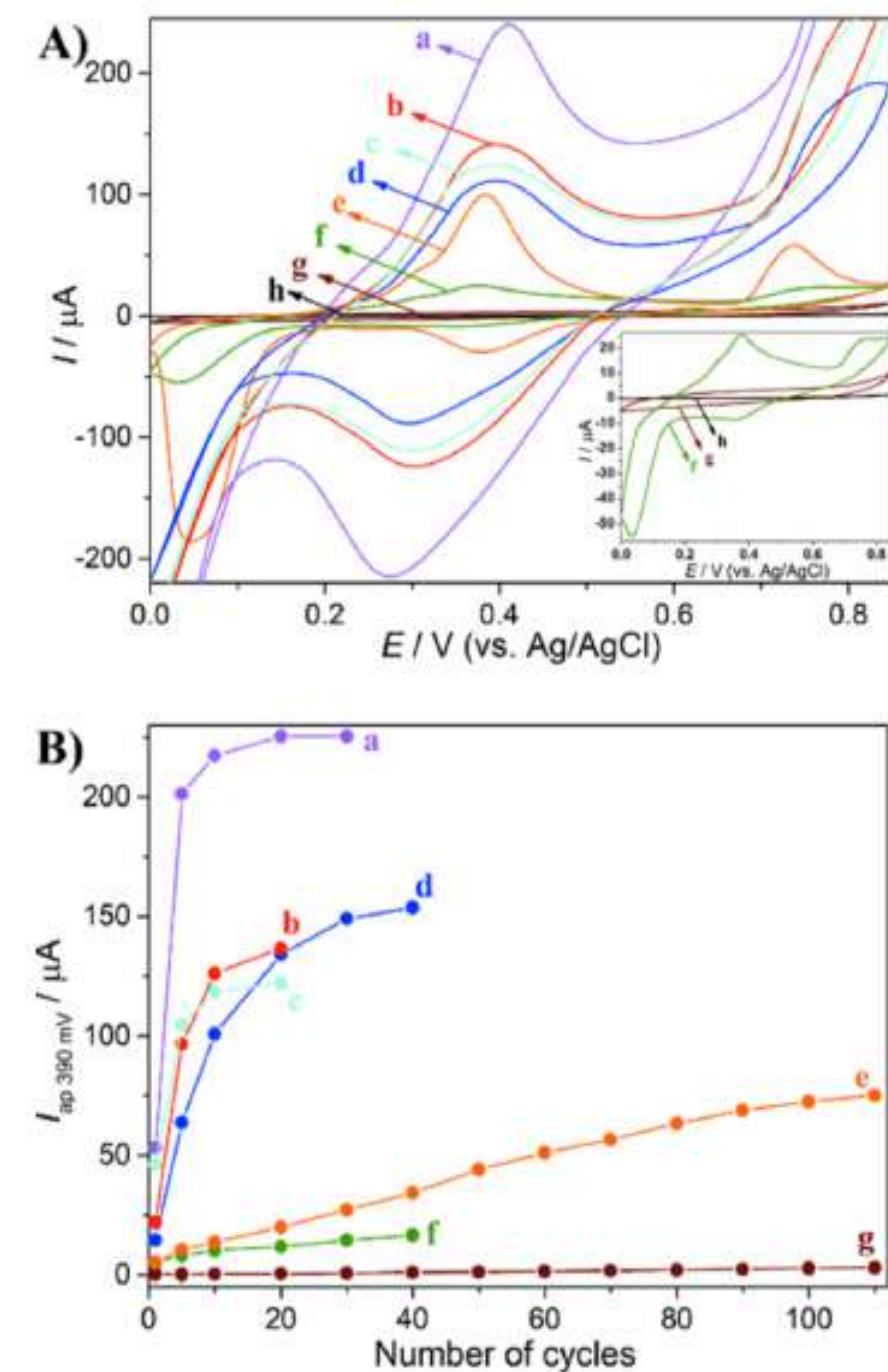
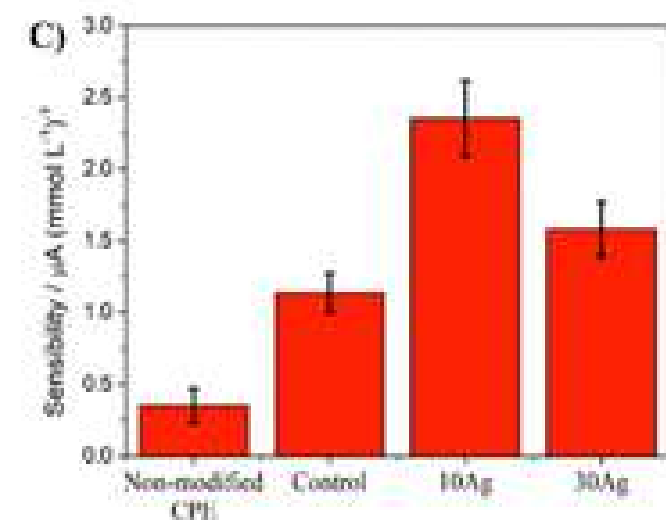
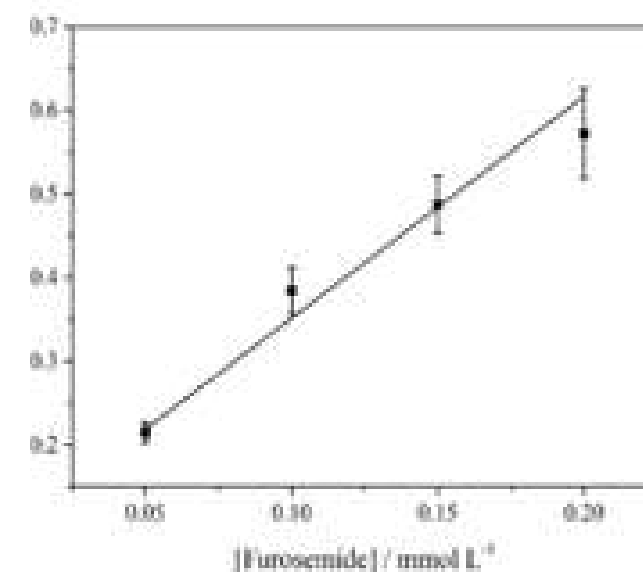
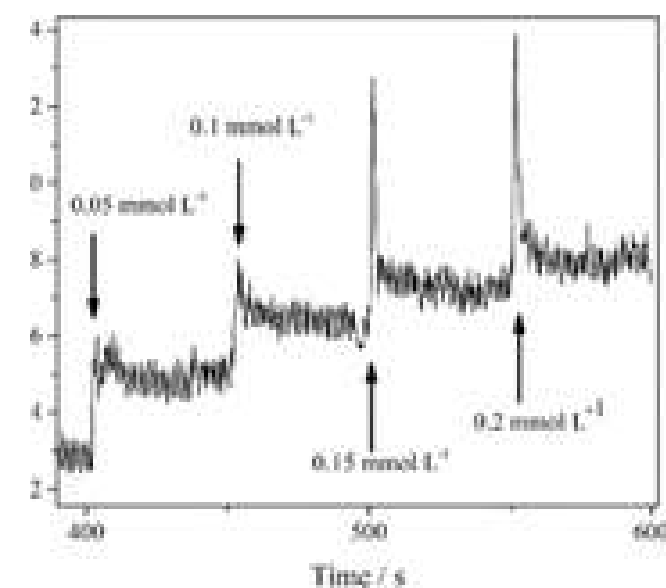
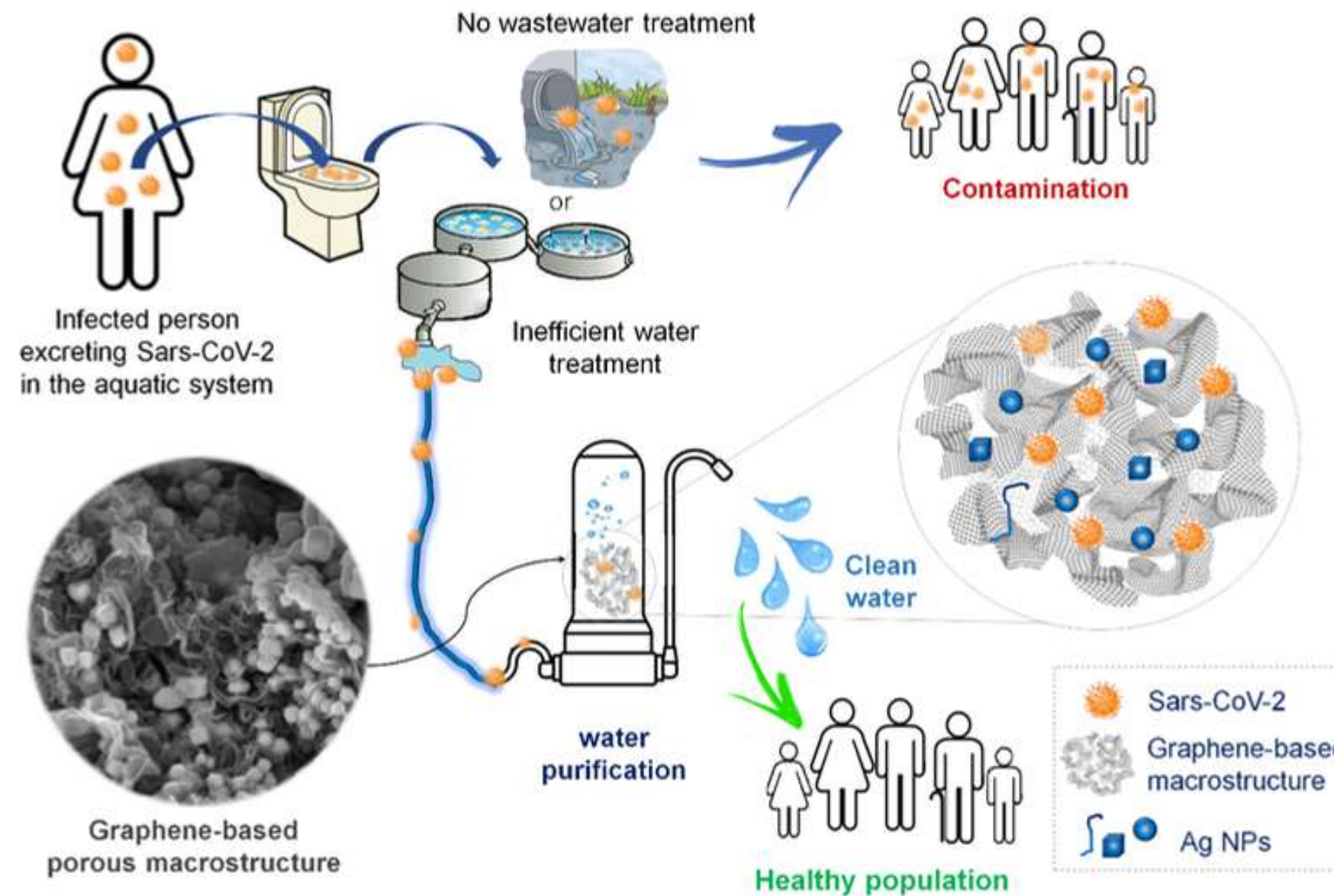


Figure 7. (A) Cyclic voltammograms and (B) anodic peak current at ~ 0.390 V as a function of cycling of (a) 10Ag + CTAB, (b) CTAB + 30Ag, (c) 30Ag + CTAB, (d) CTAB + 10Ag, (e) 30Ag, (f) 10Ag, (g) Control, and (h) nonmodified CPE. The inset in A shows the cyclic voltammograms magnified. The cyclic voltammograms were collected in an aqueous solution of 0.1 mol L^{-1} KOH at 50 mV s^{-1} .

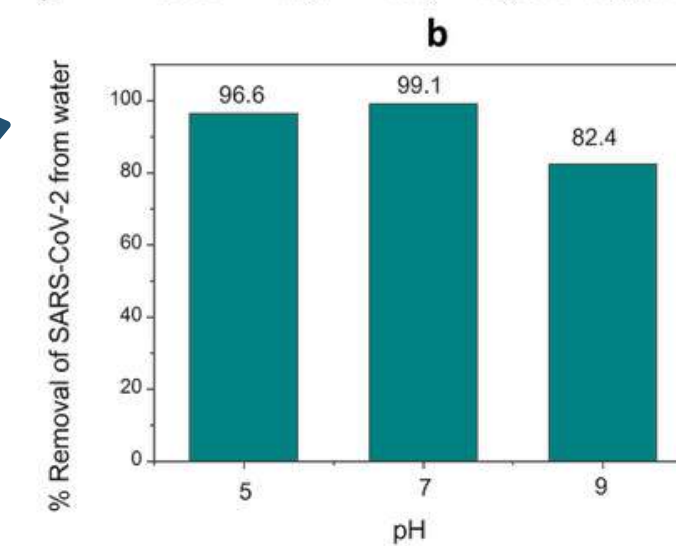
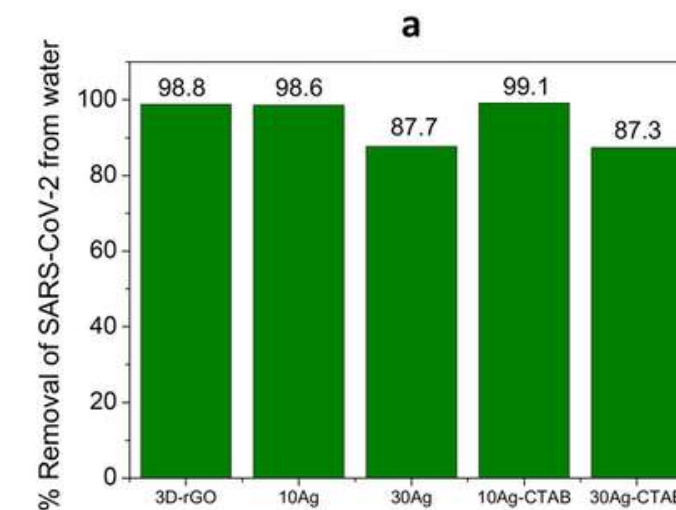
Virus



Sars-Cov2



**RODRIGO VOUCHER GROUP
CCQFA (UFPEL)**



P. C. C. da Rosa et al.
Submitted (2025).

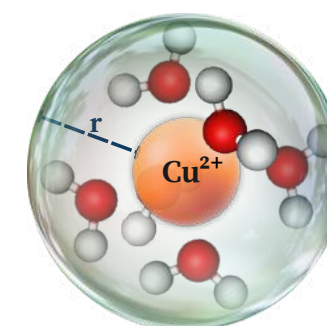
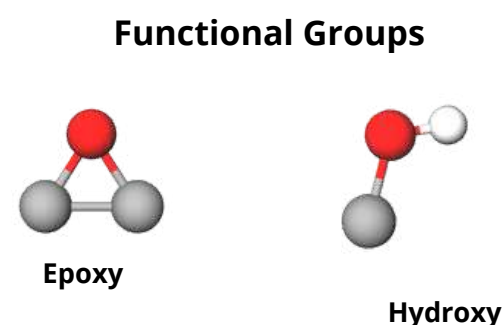
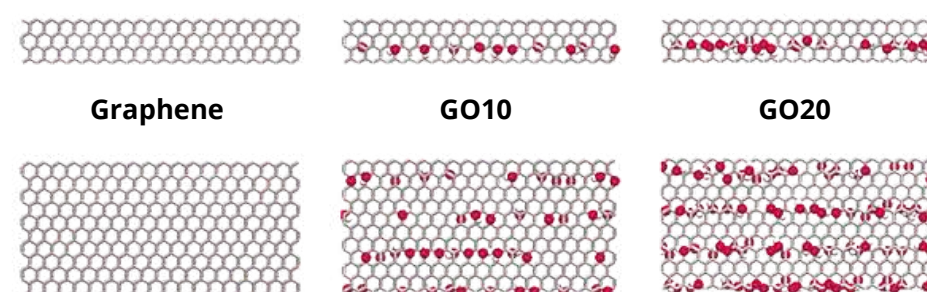
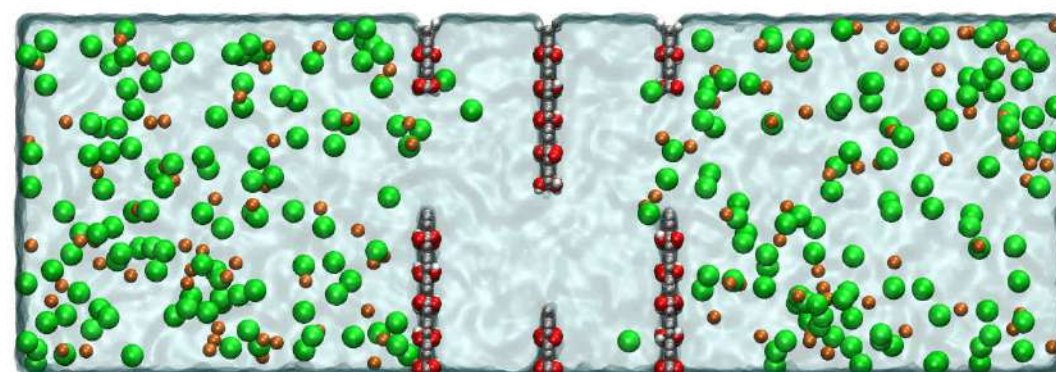


Heavy Metals

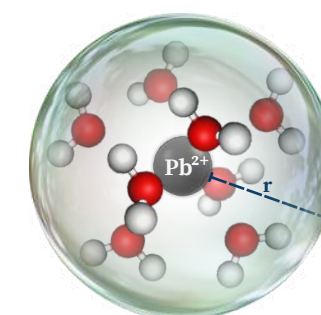
Copper and Lead



● Oxygen ● Carbon ● Copper
● Hydrogen ● Chlorine ● Lead



Coordination number
 5.71 ± 0.02



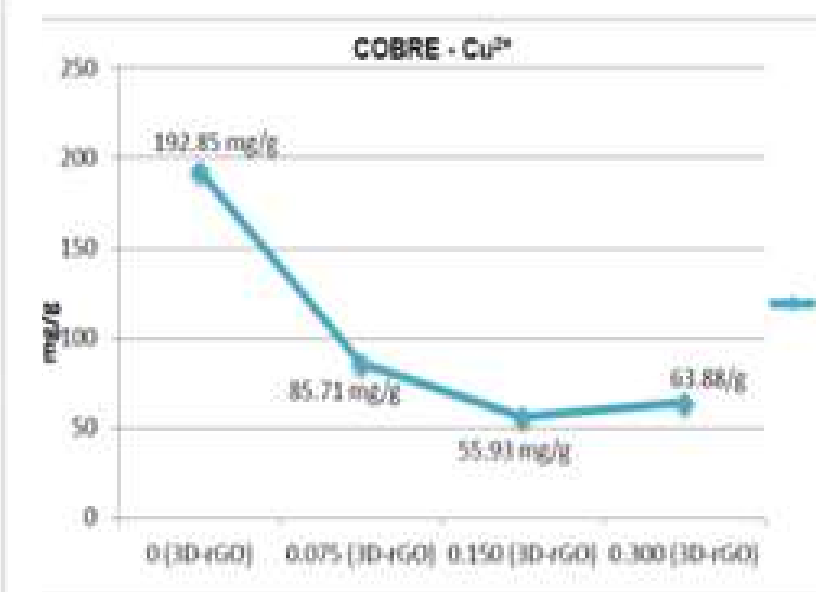
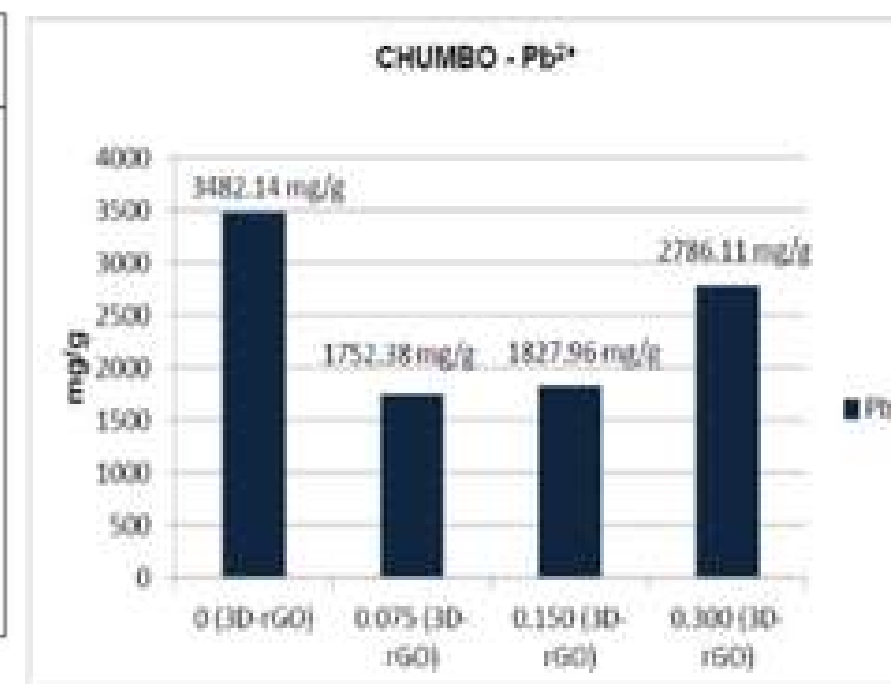
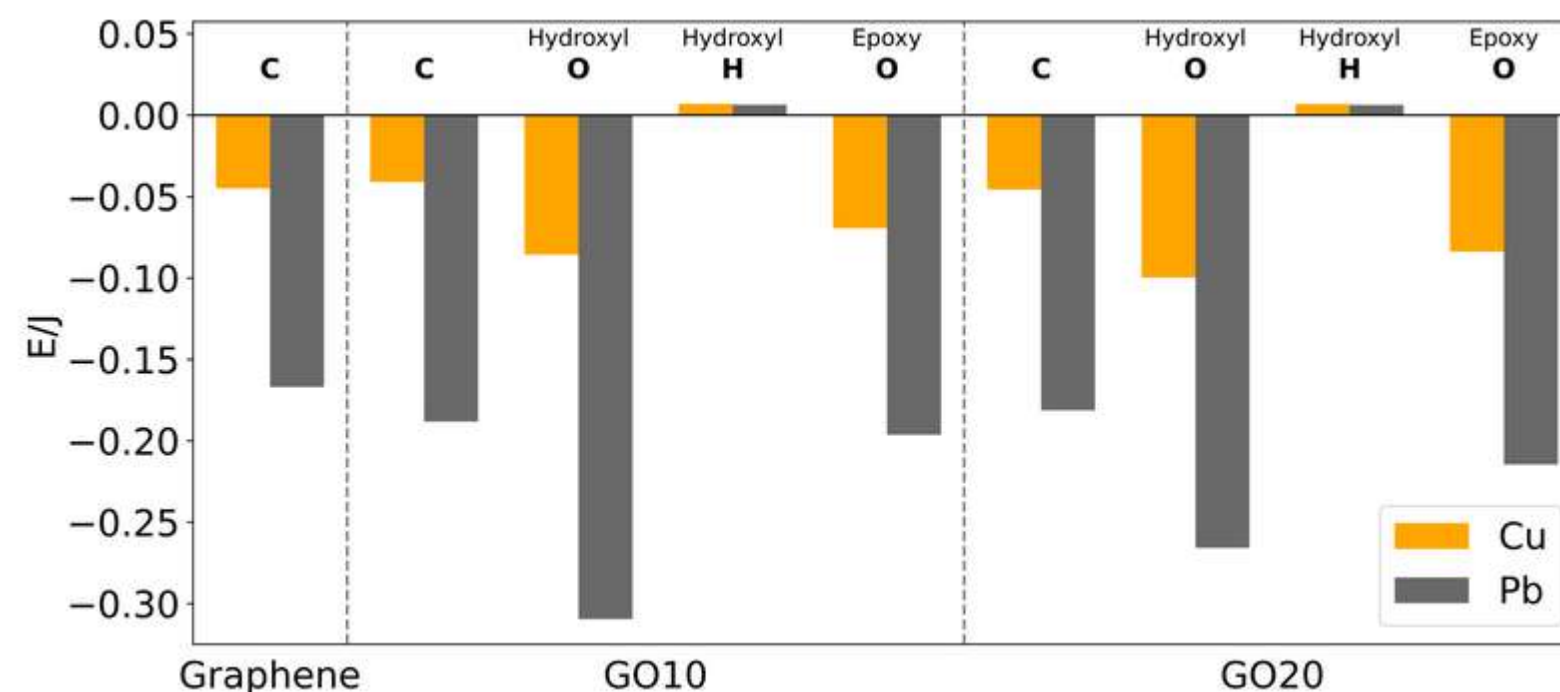
Coordination number
 7.81 ± 0.02



PATRICK CORTES
PHD (UFPEL)



MATEUS H. KÖHLER
LABORATÓRIO
COMPUTACIONAL DE
NANOMATERIAIS (UFMS)



Nanoscale water behavior and its impact on adsorption: A case study with CNTs and diclofenac

Cite as: J. Chem. Phys. 162, 034701 (2025); doi: 10.1063/5.0246155

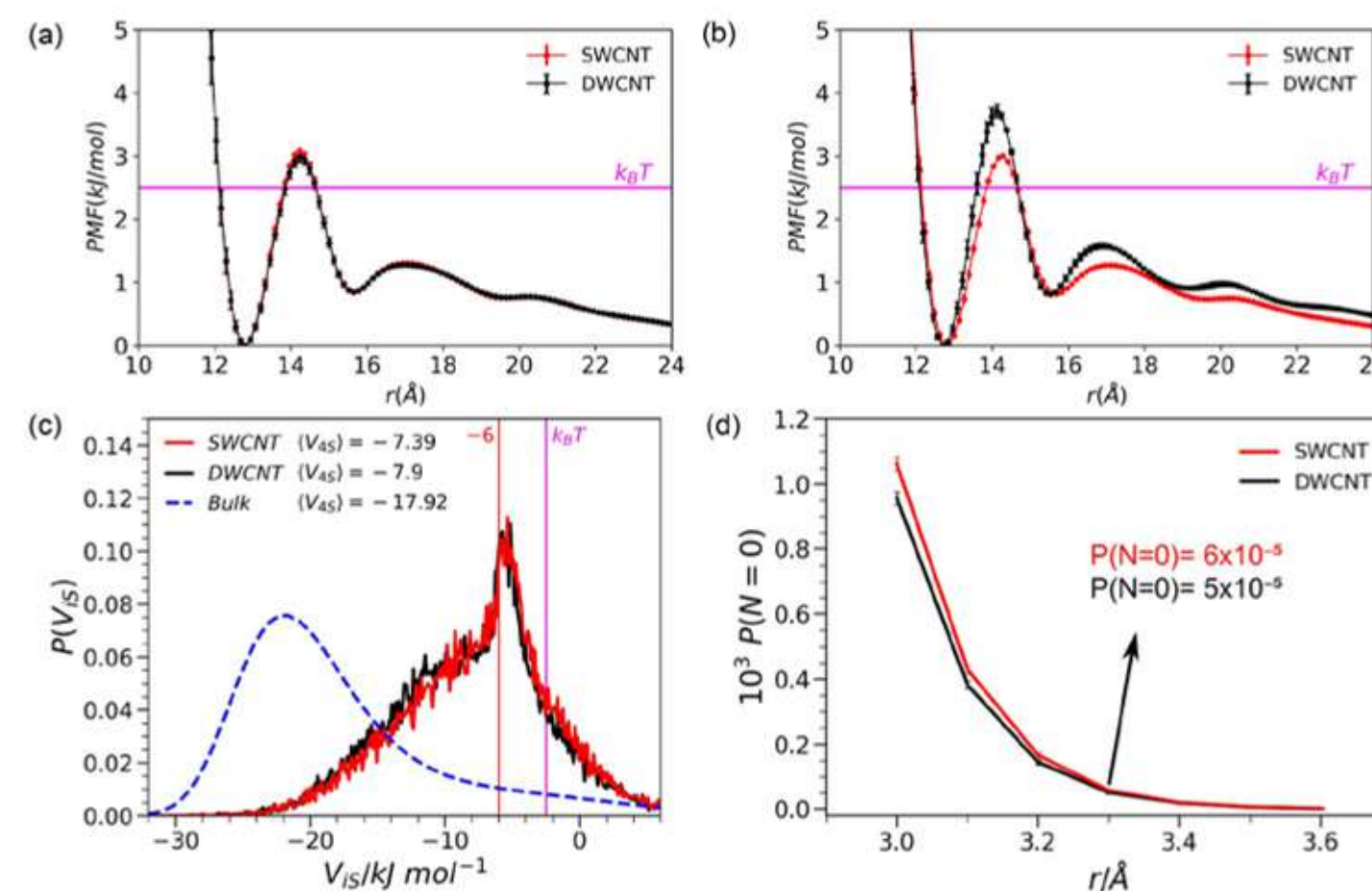
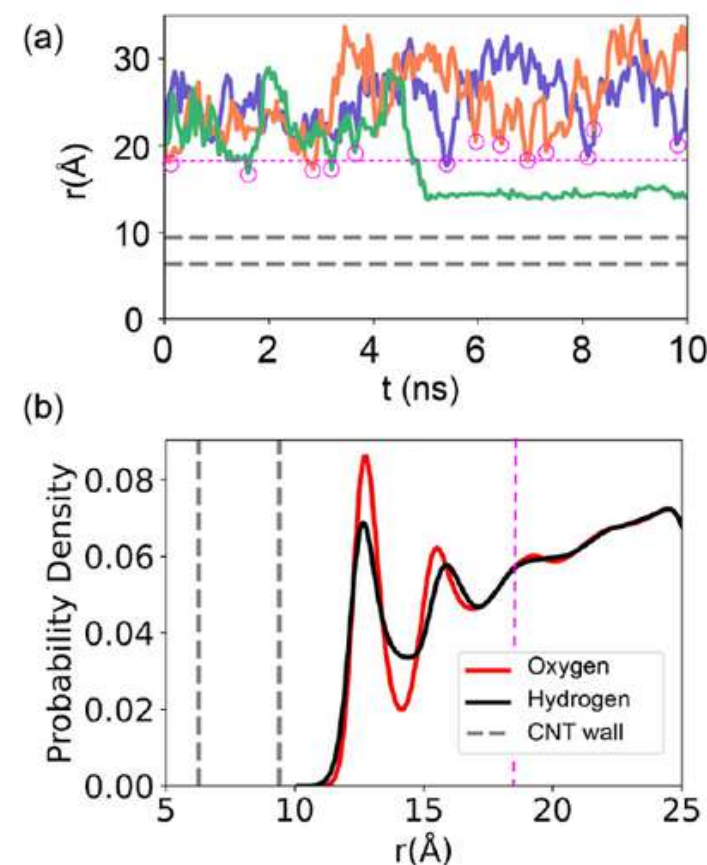
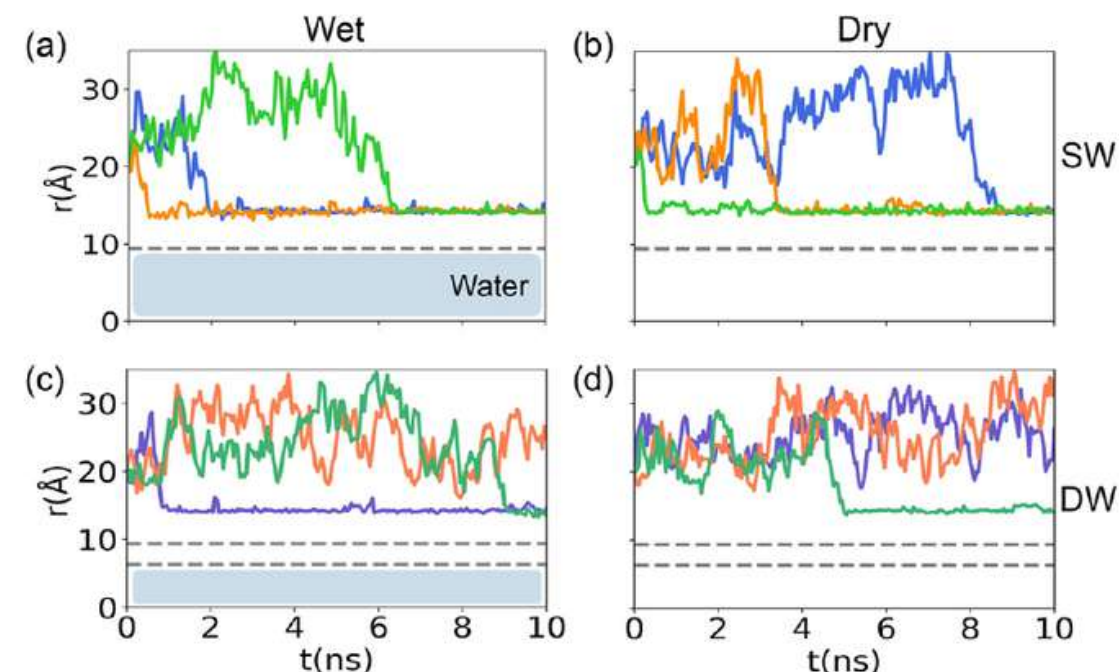
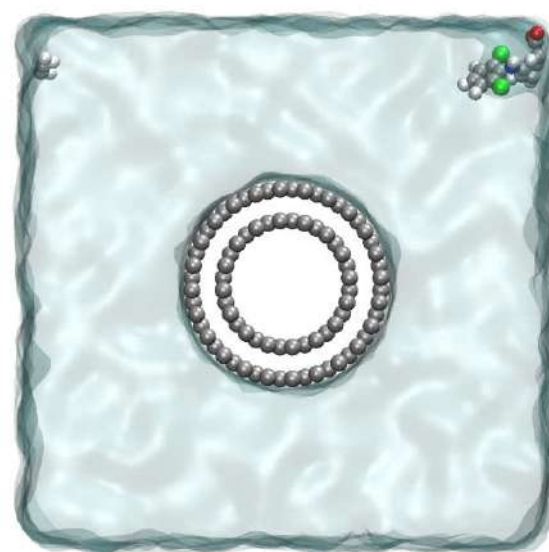
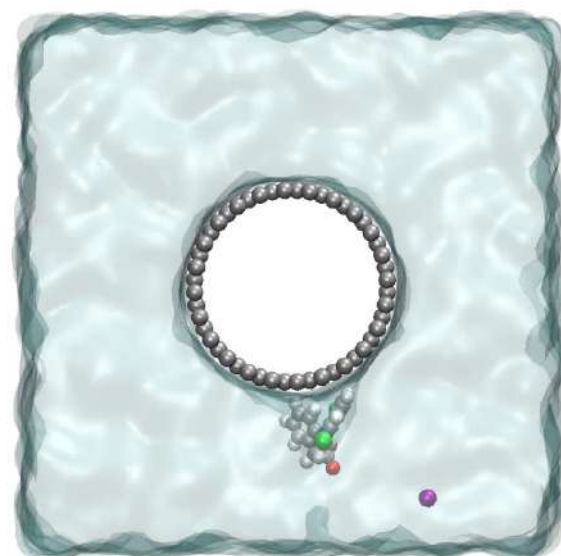
Submitted: 30 October 2024 • Accepted: 4 December 2024 •

Published Online: 15 January 2025

Patrick R. B. Côrtes,¹ Nicolás A. Loubet,² Luana S. Moreira,³ Cintia A. Menéndez,² Gustavo A. Appignanesi,² Mateus H. Köhler,^{2,3} and José Rafael Bordin^{1,3}



Gustavo Appignanesi Group
INQUISUR - UNS/Argentina



Oil

design of nanorods (back to theory)



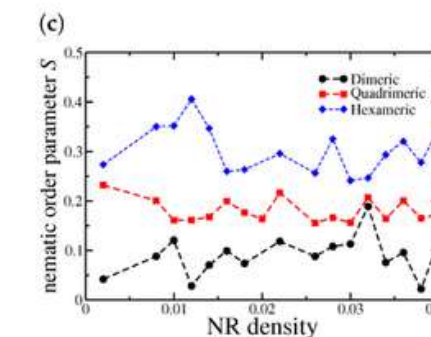
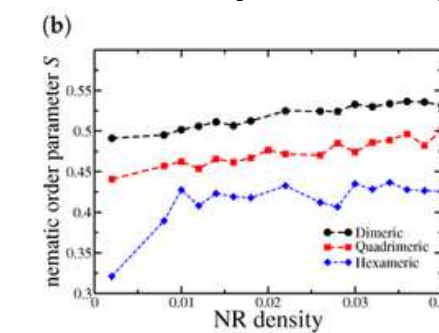
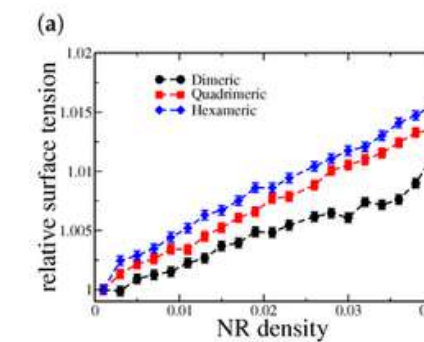
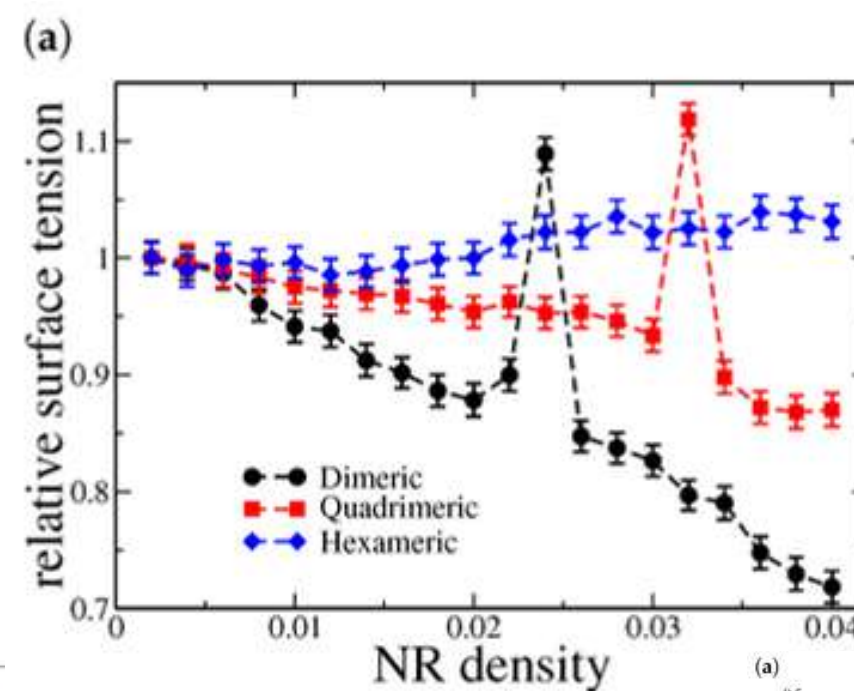
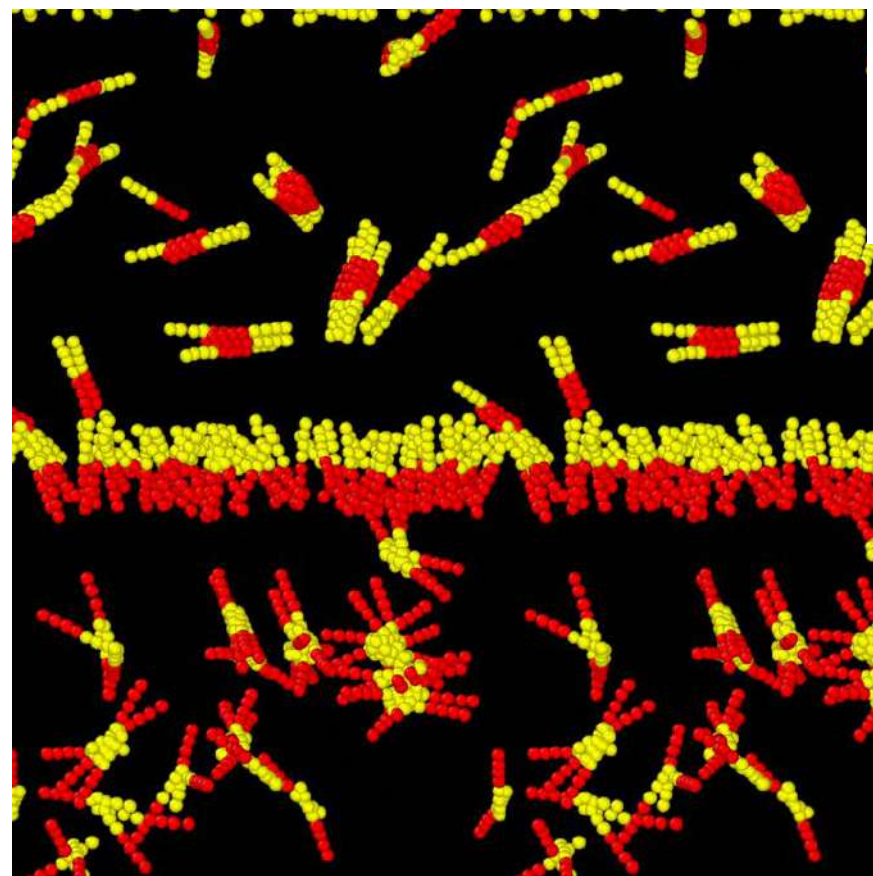
ALEXSANDRA DOS SANTOS
PHD (UFPEL)



Article

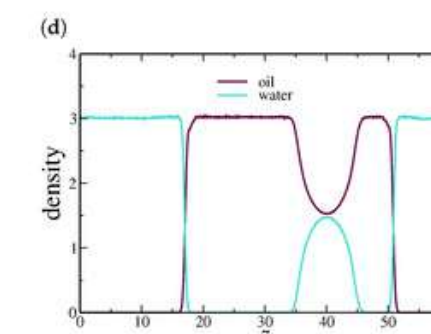
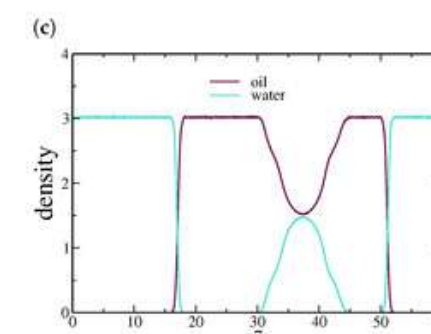
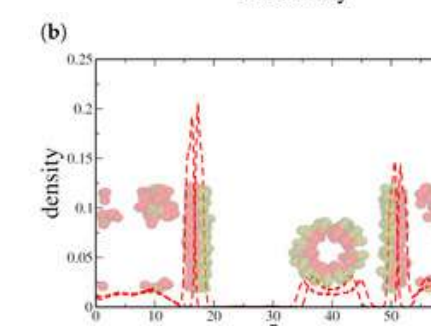
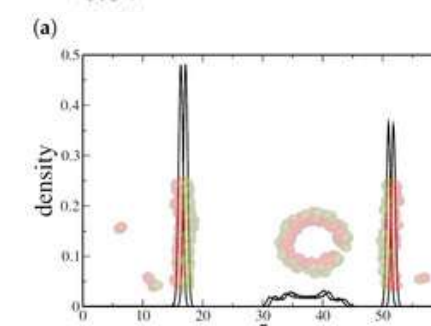
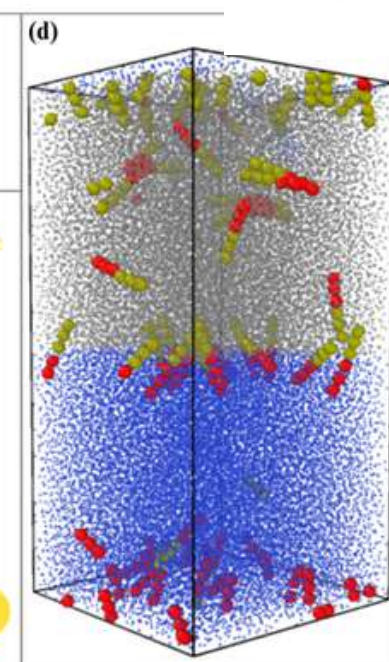
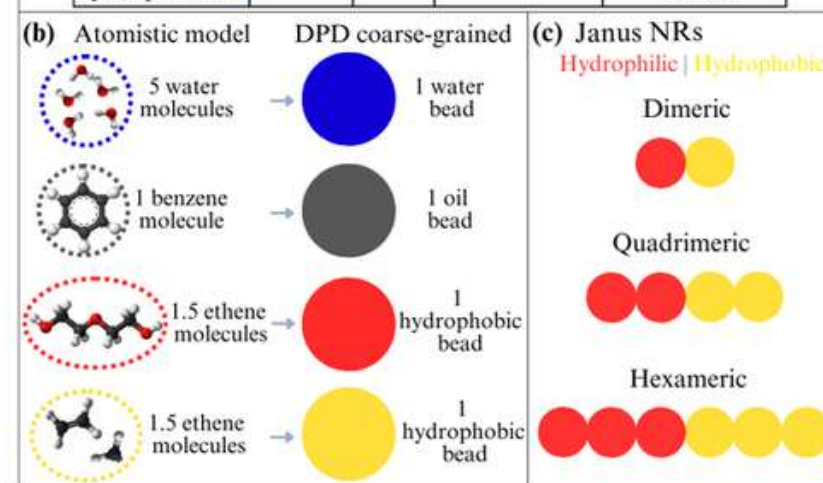
Interfacial Behavior of Janus Nanorods: A Dissipative Particle Dynamics (DPD) Study on Water–Oil Systems and Nanoconfinement

Alexsandra Pereira dos Santos ¹, Carolina Ferreira de Matos Jauris ² and José Rafael Bordin ^{1,*}



(a)

	water	oil	hydrophilic	hydrophobic
water	131.50	171.43	0.00	168.90
oil		131.50	142.07	132.08
hydrophilic			131.50	140.83
hydrophobic				131.50



and also...

design of hairy balls (back to theory & experiment)



new: gold nanospheres decorated with ionic liquids



ENRIQUE LOMBA
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BLAS CABRERA E
UNIVERSIDADE DE SANTIAGO
DE COMPOSTELA/ESPANHA

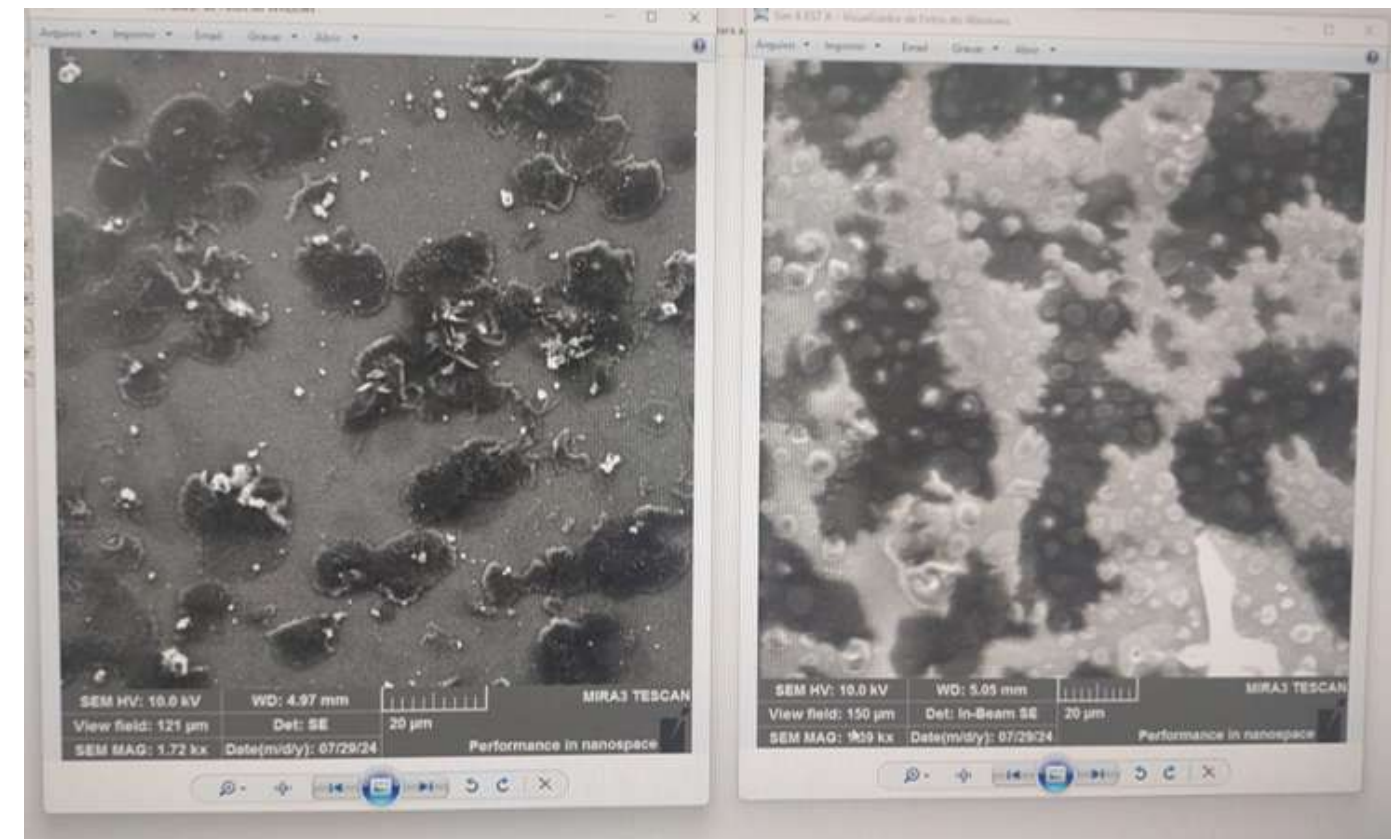
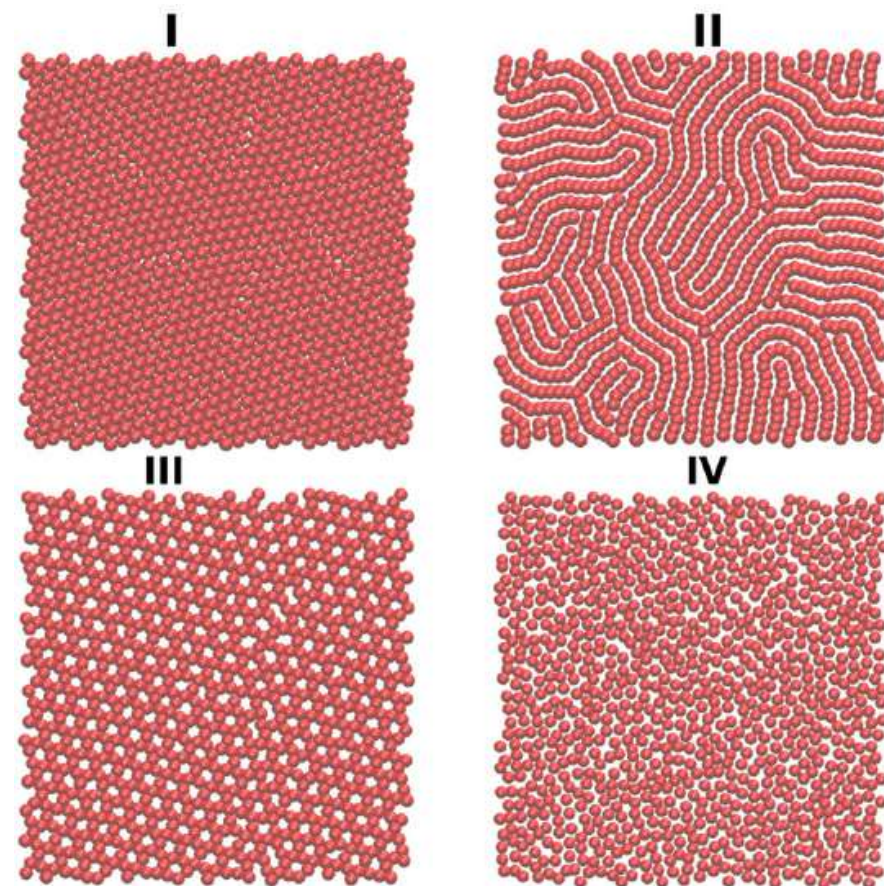
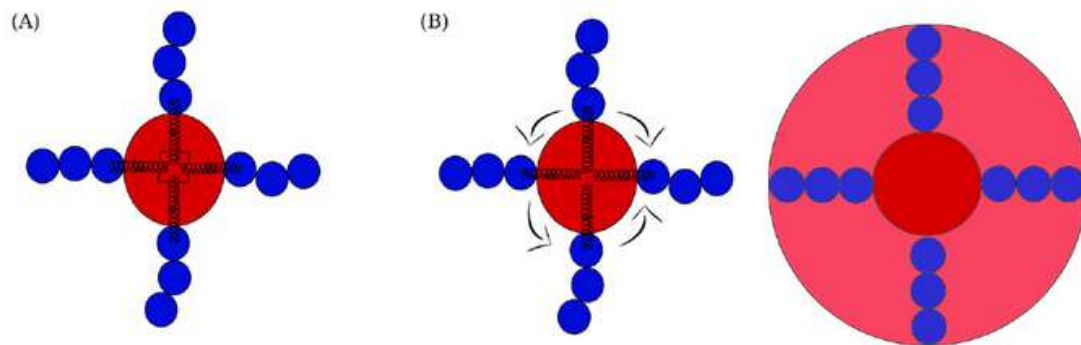
WATER AT NANOSCALE

Journal of
Applied Physics

Waterlike anomalies in hard core-soft shell nanoparticles using an effective potential approach: Pinned vs adsorbed polymers

Cite as: J. Appl. Phys. 127, 054701 (2020); <https://doi.org/10.1063/1.5128938>
Submitted: 23 September 2019 . Accepted: 20 January 2020 . Published Online: 04 February 2020

Murilo S. Marques , Thiago P. O. Nogueira, Rodrigo F. Dillenburg, Marcia C. Barbosa , and José Rafael Bordin





1. The Physics of Nanoconfined Water is Key to Understanding and Controlling Processes in Nanotechnology and Environmental Safety

- Understanding water behavior at the nanoscale reveals unique phenomena absent in bulk systems, serving as a foundation for designing efficient solutions across fields from biotechnology to environmental engineering.

2. From Fundamental Knowledge to Practical Impact: Basic Science Drives Innovation

- Theoretical studies and molecular simulations help unravel adsorption mechanisms and interactions, guiding the rational design of advanced nanomaterials to tackle real-world challenges like emerging contaminant removal.

3. Smart Nanomaterials are the Future of Environmental Remediation

- By combining tunable nanomaterial properties with molecular-level insights, we can develop more selective, efficient, and sustainable technologies for water treatment.

4. Interdisciplinarity is Essential: Where Physics Meets Engineering and Sustainability

- Addressing complex issues such as water scarcity and pollution by emerging contaminants requires integrated approaches—bringing together physics, chemistry, materials science, and environmental concerns to transform knowledge into practical solutions.

Water Air Soil Pollut (2023) 234:136
<https://doi.org/10.1007/s11270-023-06146-6>

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

Mayara Bitencourt Leão · José Rafael Bordin ·
 Carolina Ferreira de Matos



IOP Publishing

J. Phys.: Condens. Matter 37 (2025) 113004 (21pp)

Journal of Physics: Condensed Matter

<https://doi.org/10.1088/1361-648X/ada65b>

Topical Review

**Computational condensed matter
 science contributions to addressing
 water emerging contaminant pollution:
 a comprehensive review**

José Rafael Bordin^{1,*}, Carolina Ferreira de Matos Jauris², Patrick R B Côrtes¹,
 Wanderson S Araújo¹, Luana S Moreira³, Alessandra Pereira dos Santos¹,
 Mayara Bitencourt Leão⁴, Elizane E Moraes⁵, Maurício J Piotrowski¹
 and Mateus H Köhler³

Concluding



Take-Home Messages



“La utopía está en el horizonte. Camino diez pasos y ella se aleja diez pasos, camino veinte pasos y ella se corre veinte pasos más allá. ¿Entonces para qué sirve la utopía? Para eso, sirve para caminar”

Fernando Birri/Eduardo Galeano

“The academy is not paradise. But learning is a place where paradise can be created”

Bell Hooks

“Minha esperança é necessária mas não é suficiente. Ela, só, não ganha a luta, mas sem ela a luta fraqueja e titubeia.”

Paulo Freire

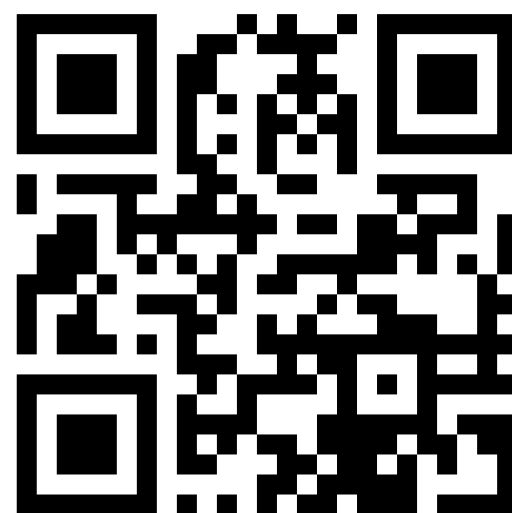
WITHOUT PUBLIC FUNDING THIS RESEARCH WOULD BE IMPOSSIBLE



Concluding



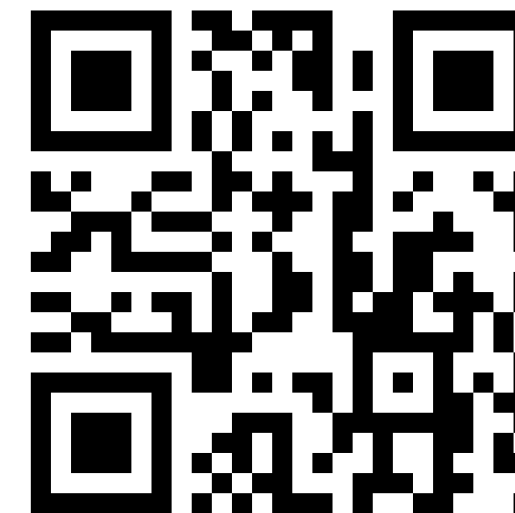
Obrigado! Thanks! Gracias!



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