Ciclo de palestras sobre Astrobiologia

Física da Matéria Mole:
da nanoescala ao centro de galáxias

José Rafael Bordin
Departamento de Física
Universidade Federal de Pelotas

BORDIN LAB
SOFT MATTER PHYSICS

Sumário

→ O que é Matéria Mole?

→ Como estudamos?

→ Nanofluídica & Coloides & Nanomateriais

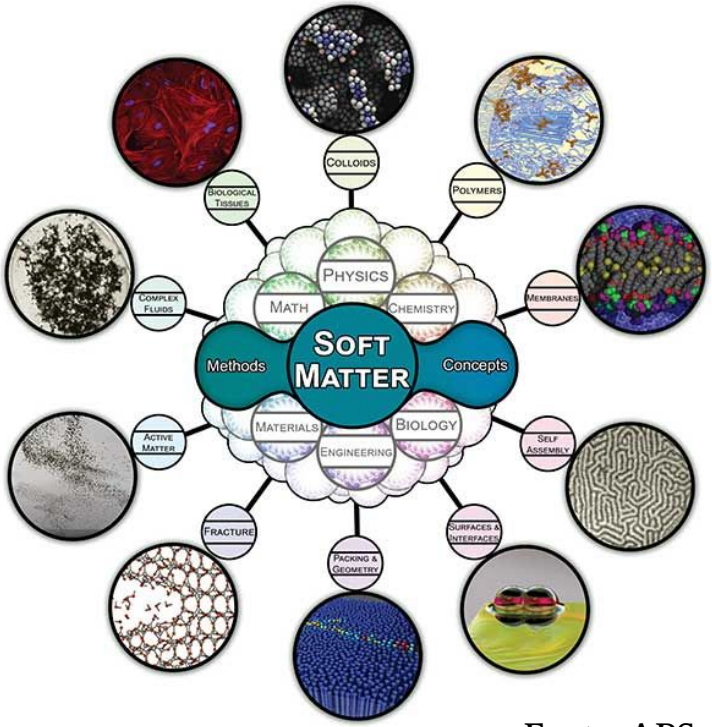
[classical leap]

→ Sistemas Biológicos

[quantum leap]

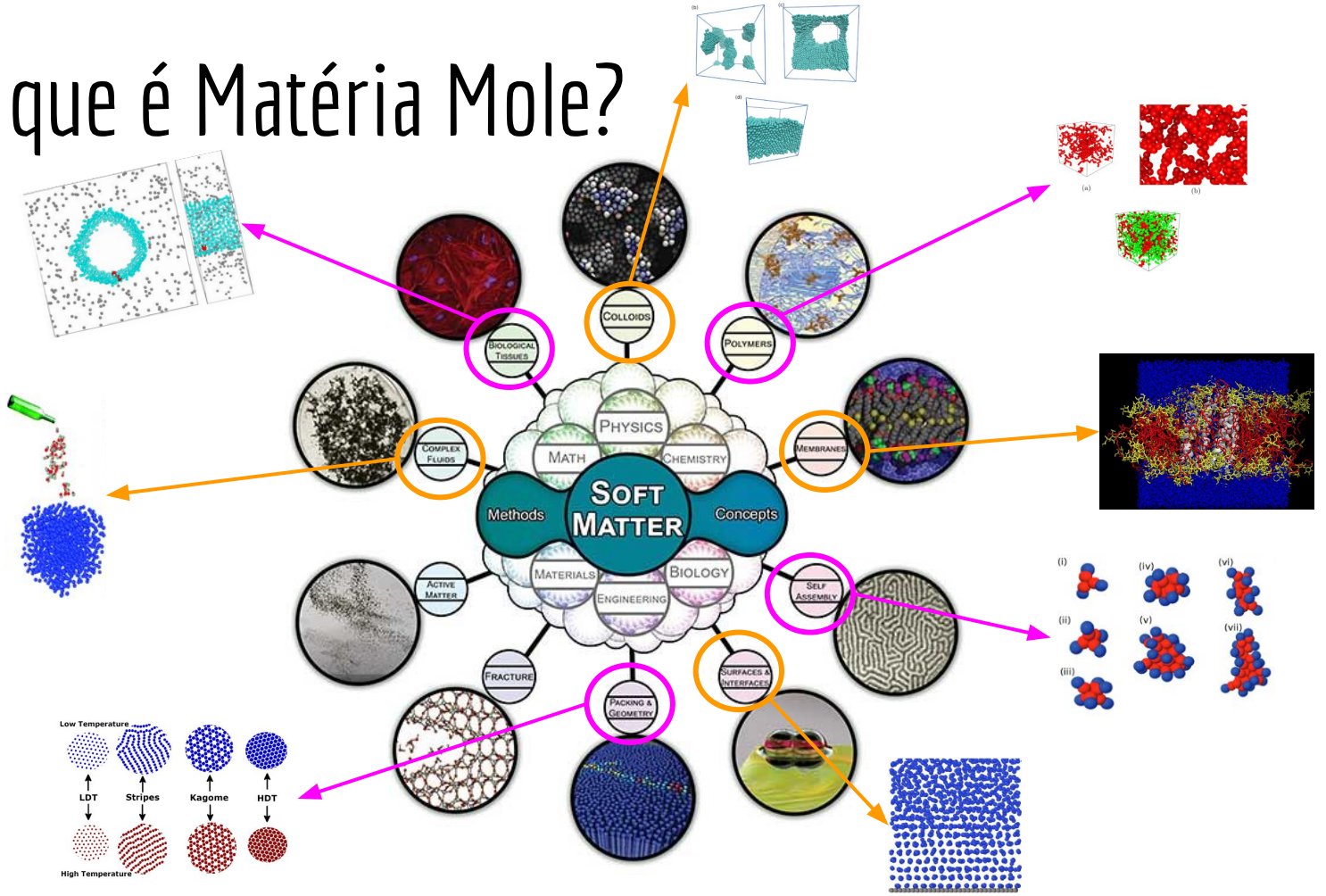
→ PAHs no Centro de Galáxias

O que é Matéria [Condensada] Mole?



Fonte: APS

O que é Matéria Mole?



Ninguém pesquisa sozinho

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Lucas Avila Pinheiro
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Milena Costa Guidotti
Lattes milenaguidotti@gmail.com

Mais ex-alunos de Doutorado, Mestrado e IC que não cabem aqui

Colaborações:

⟶ Marcia C. Barbosa (UFRGS)

⟶ Carolina Jauris (Unipampa)

⟶ Mateus Kohler (UFSM)

⟶ Dinalva Aires de Sales (FURG)

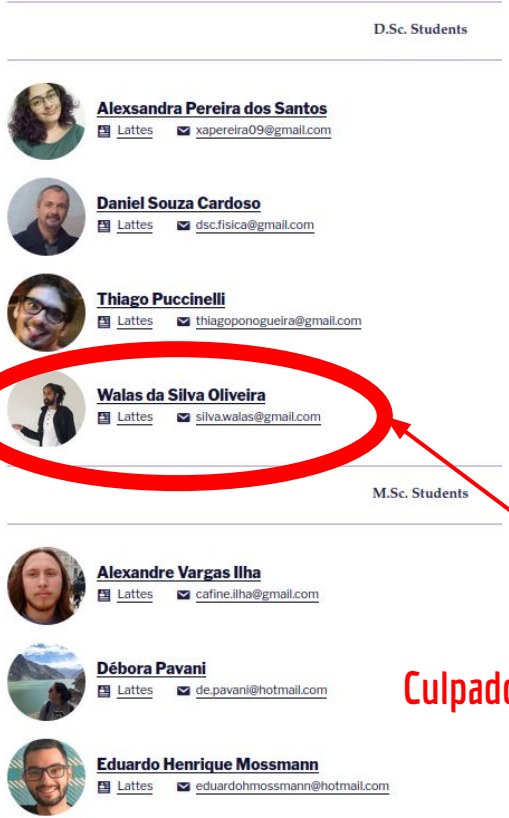
⟶ Francesco Piazza (Uni. Florença)

⟶ Mauricio Moreira-Soares (Uni. Oslo)

⟶ Rui Travasso (Uni. Coimbra)

⟶ Aqui vão todos que não incluí por falta de espaço

Ninguém pesquisa sozinho



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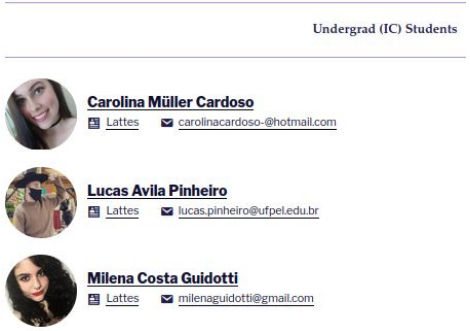

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Milena Costa Guidotti
Lattes milenaguidotti@gmail.com

Culpados por eu estar aqui hoje

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→ Rui Travasso (Uni. Coimbra)

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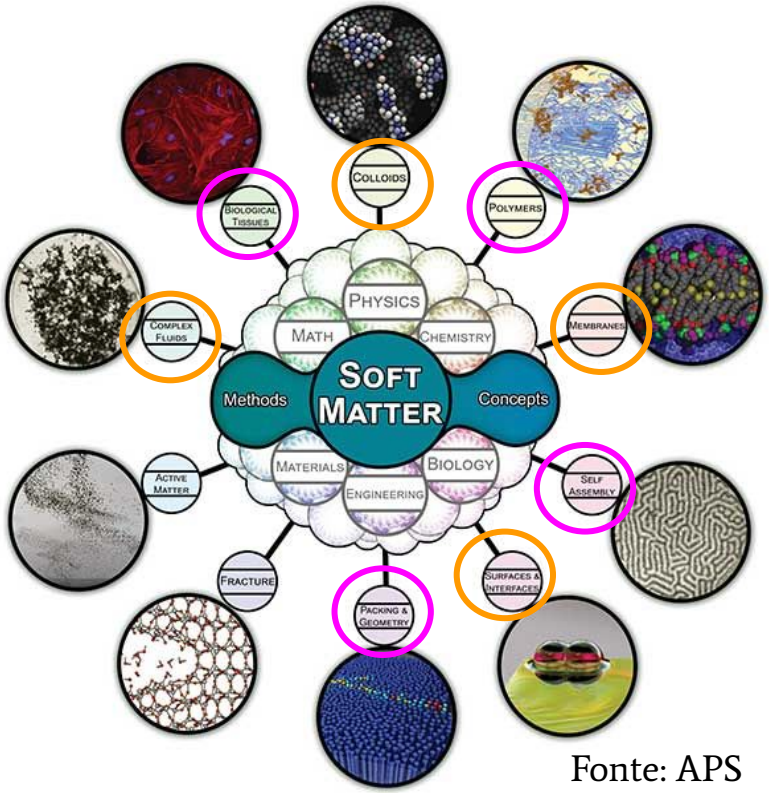
Como nós estudamos Matéria Mole?



Fonte: APS

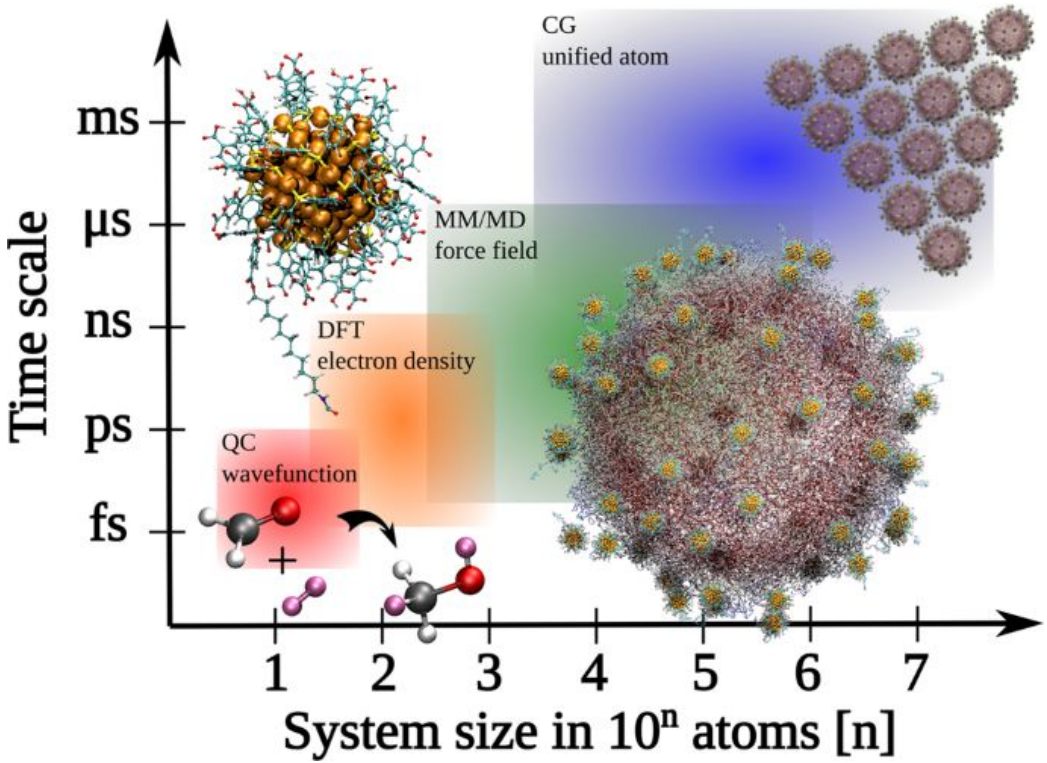
MODELAGEM

MOLECULAR

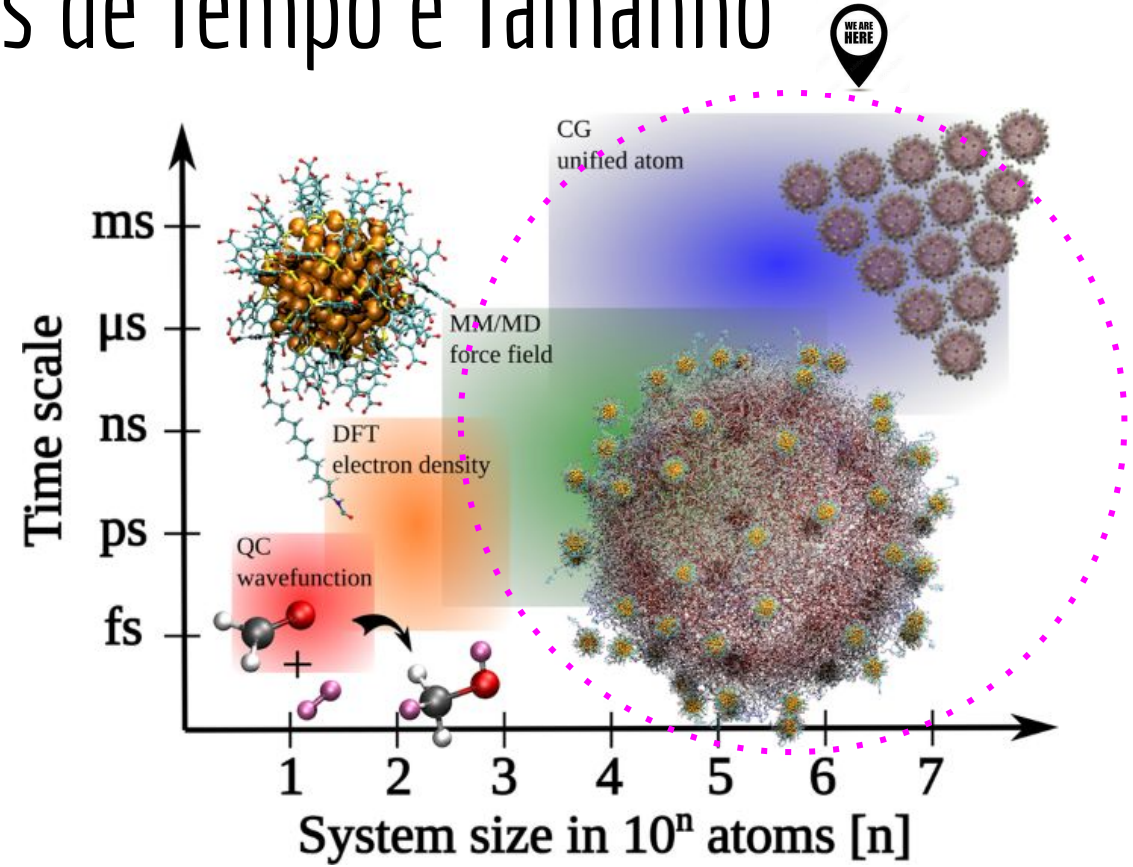
Relações entre

- dinâmica
- termodinâmica
- estrutura
- COMPETIÇÕES

Escalas de Tempo e Tamanho

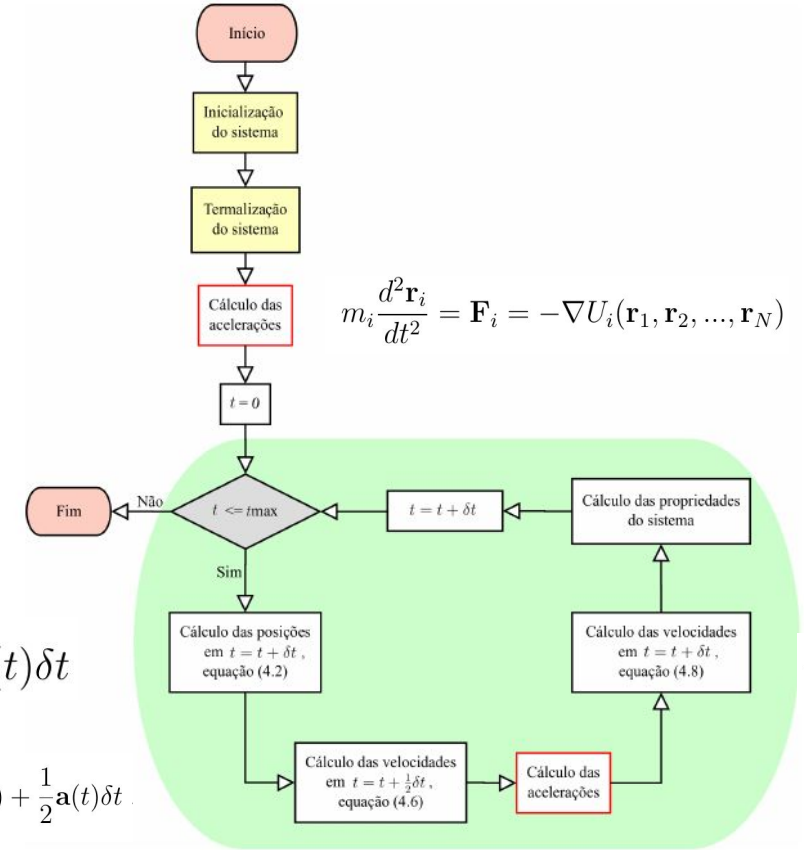


Escalas de Tempo e Tamanho



Dinâmica Molecular [Clássica]

(ou MRUV com nome chique)



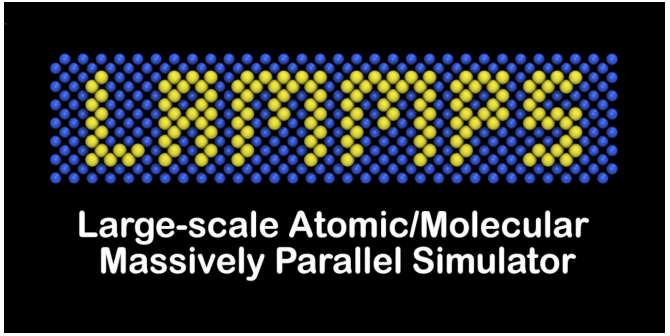
$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{F}_i = -\nabla U_i(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$$

$$\mathbf{r}(t+\delta t) = \mathbf{r}(t) + \mathbf{v}(t)\delta t$$

$$\mathbf{v}\left(t+\frac{1}{2}\delta t\right) = \mathbf{v}(t) + \frac{1}{2}\mathbf{a}(t)\delta t$$

$$\mathbf{v}(t+\delta t) = \mathbf{v}\left(t+\frac{1}{2}\delta t\right) + \frac{1}{2}\mathbf{a}(t+\delta t)\delta t$$

Dinâmica Molecular [Clássica]

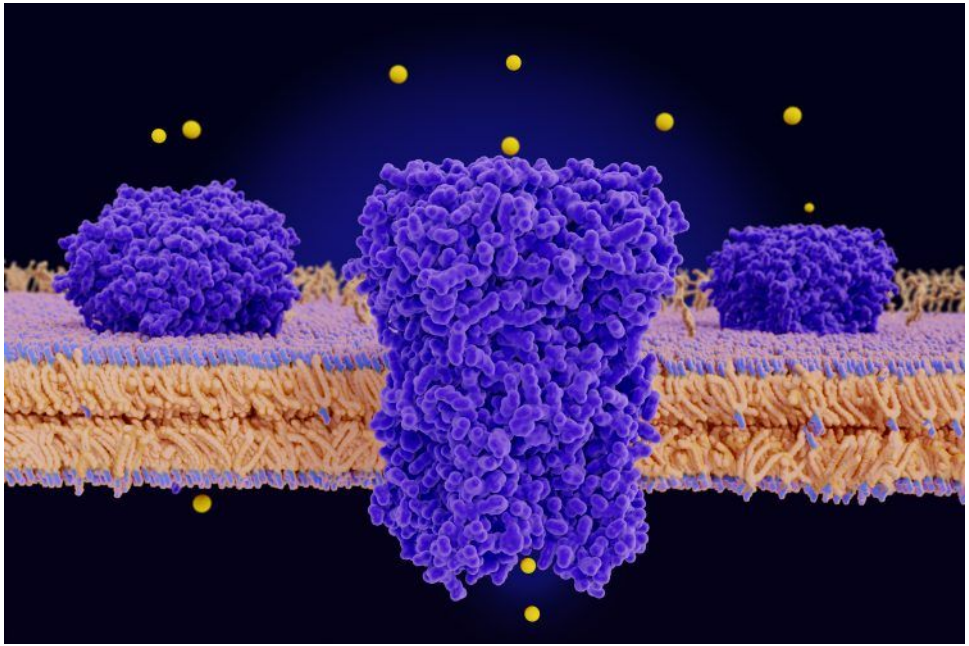


ESPResSo
An Extensible Simulation Package for Research on Soft Matter Systems
espressomd.org

lammps.org

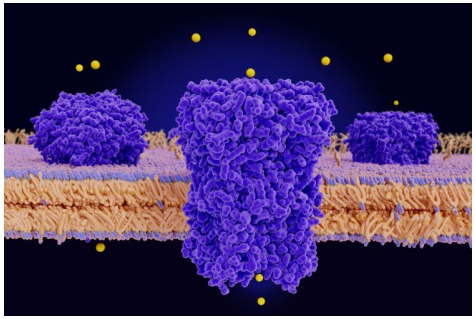
Dinâmica Molecular [Clássica]

Nanofluídica & Nanomateriais

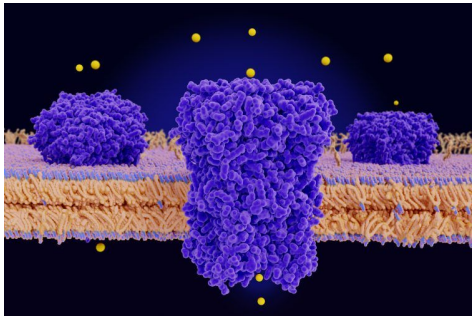


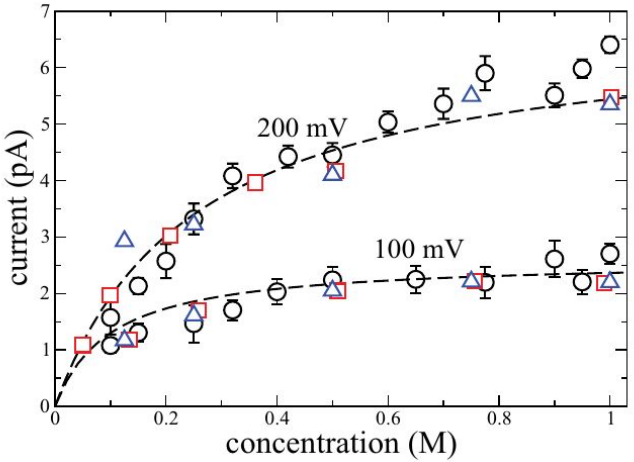
Passagem de íons em canais iônicos

Nanofluídica



Nanofluídica





PHYSICAL REVIEW E **85**, 031914 (2012)

Ion fluxes through nanopores and transmembrane channels

J. R. Bordin,[1] A. Diehl,[2] M. C. Barbosa,[3] and Y. Levin[3]

Nanofluídica

PHYSICAL REVIEW E **85**, 031914 (2012)

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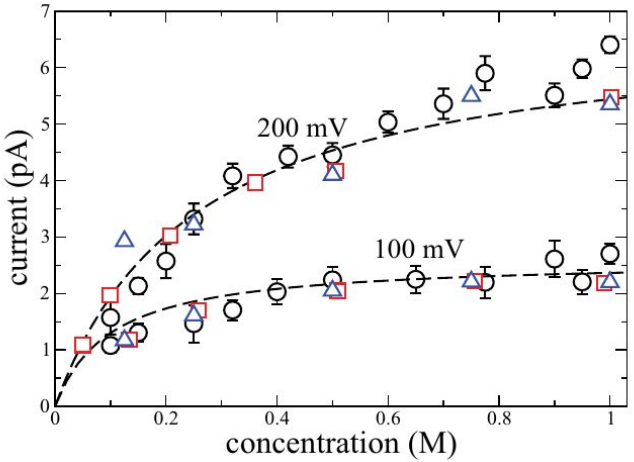
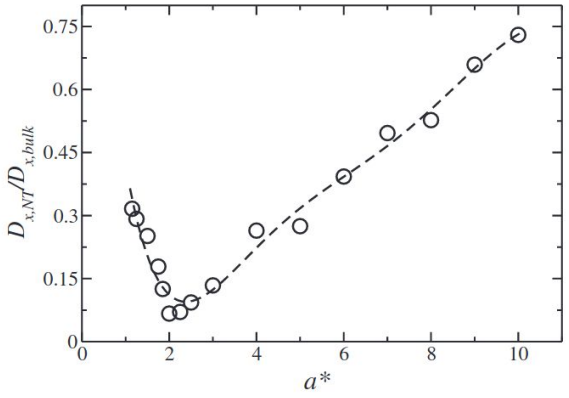
O modelo só funciona se a viscosidade dentro do canal é maior que fora (?!)

→ Estudar água nanoconfinada deve ajudar a entender isso



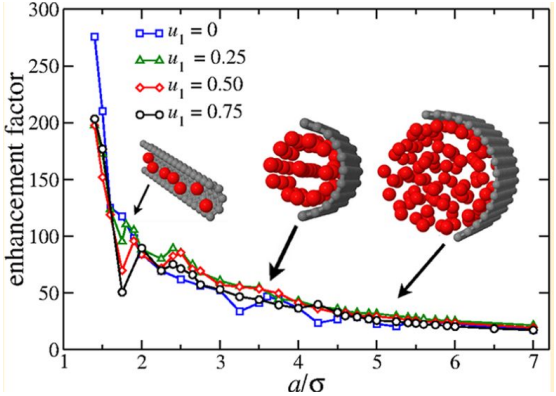
Nanofluídica



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]

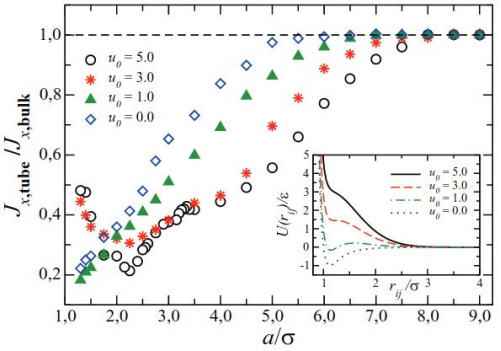


Relation Between Flow Enhancement Factor and Structure for Core-Softened Fluids Inside Nanotubes

José Rafael Bordin*, Alexandre Diehl, and Marcia C. Barbosa

View Author Information

© Cite this: *J. Phys. Chem. B* 2013, 117, 23, 7047−7056
Publication Date: May 21, 2013
https://doi.org/10.1021/jp402141f



THE JOURNAL OF CHEMICAL PHYSICS **140**, 194504 (2014)

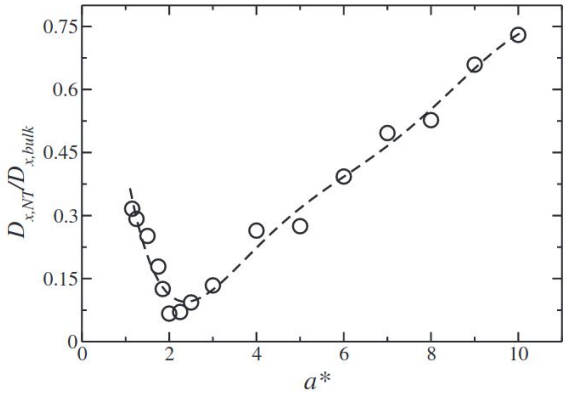
Enhanced flow of core-softened fluids through narrow nanotubes

José Rafael Bordin,[1,2,a] José S. Andrade, Jr.,[3,b] Alexandre Diehl,[2,c] and Marcia C. Barbosa[4,d]

→ Difusão, fluxo e fator de aumento de fluxo aumentam no confinamento extremo

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

Nanofluídica



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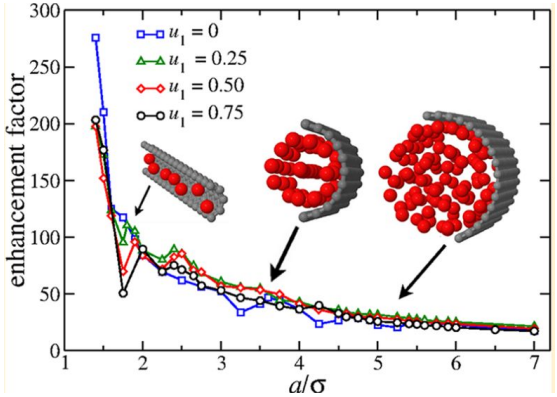

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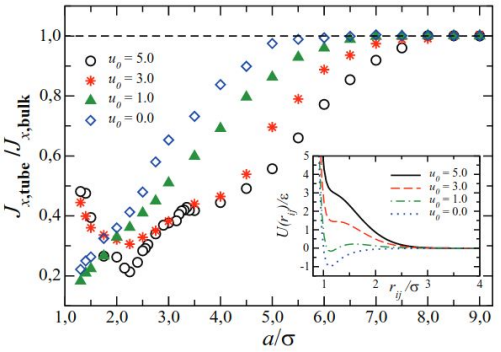

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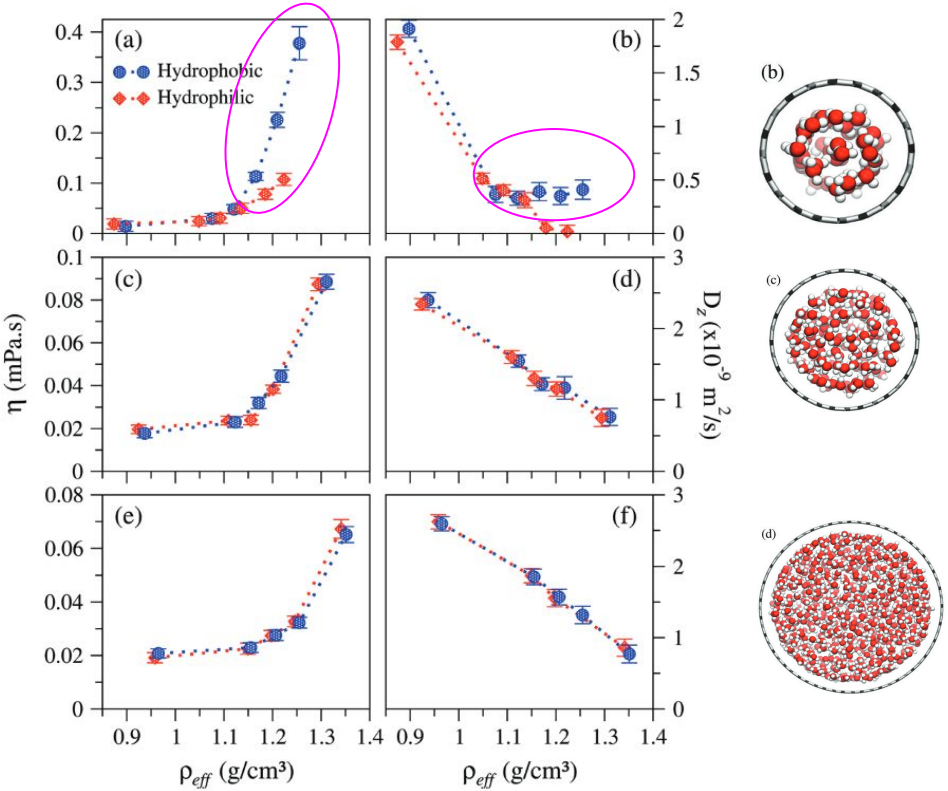
Viscosidade deve diminuir. Certo?

Nanofluídica



Viscosidade deve diminuir. Certo?

Depende...

→ Hidrofobicidade

→ Tamanho do Poro.

.

.

Check for updates

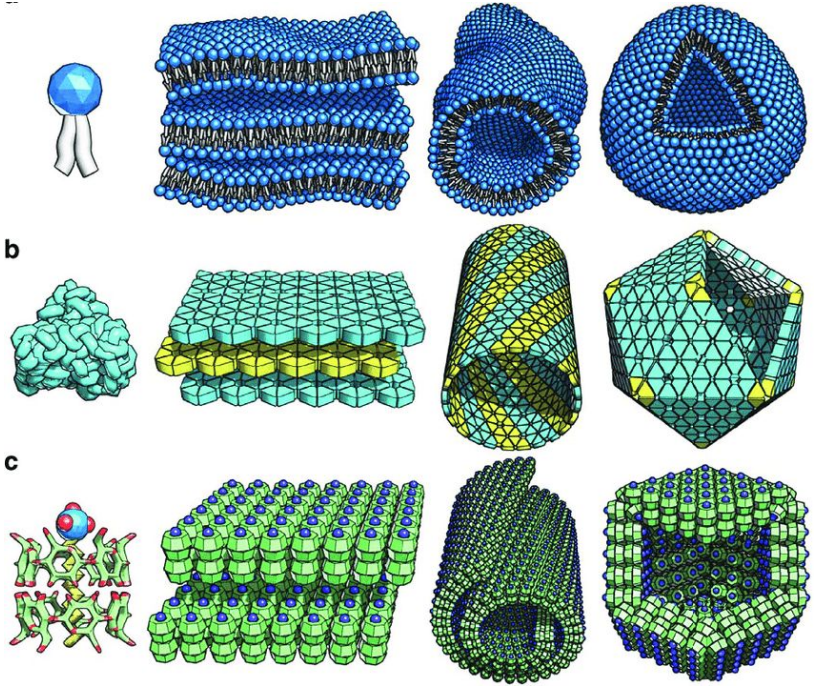
Cite this: *Phys. Chem. Chem. Phys.*, 2017, **19**, 12921

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]

Coloides & Nanomateriais

→ Self-Assembly ou Lego Molecular



Coloides & Nanomateriais

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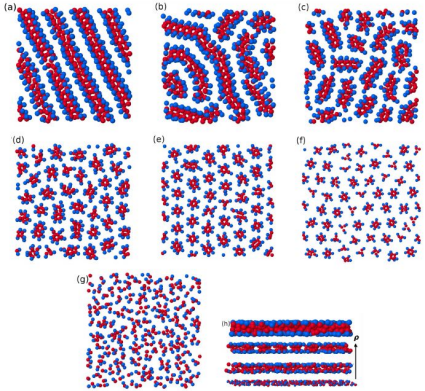
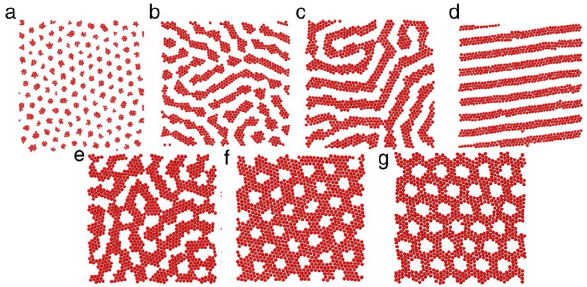


THE JOURNAL OF CHEMICAL PHYSICS **145**, 244906 (2016)

Anomalous diffusion and diffusion anomaly in confined Janus dumbbells

Leandro B. Krott,[1,a)] Cristina Gavazzoni,[2] and José Rafael Bordin[3,b)]



Physica A 495 (2018) 215–224

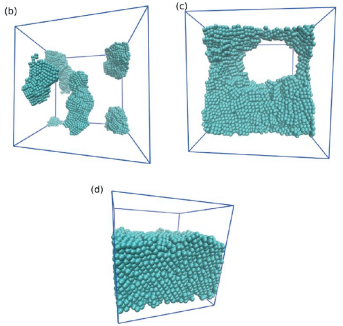
Contents lists available at ScienceDirect

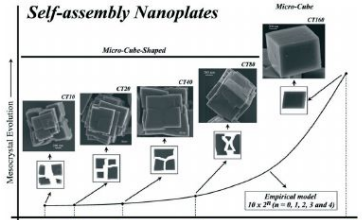
Physica A

journal homepage: www.elsevier.com/locate/physa

Distinct aggregation patterns and fluid porous phase in a 2D model for colloids with competitive interactions

José Rafael Bordin



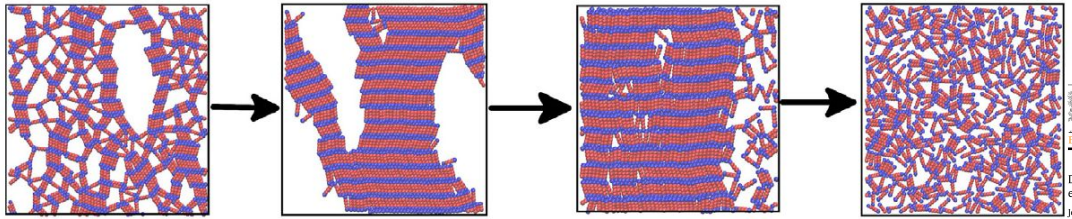


Check for updates

Cite this: *Mol. Syst. Des. Eng.*, 2020, 5, 1255

A description of the formation and growth processes of $CaTiO_3$ mesocrystals: a joint experimental and theoretical approach†

Mario L. Moreira,[a] José Rafael Bordin,[*a] Juan Andrés,[b] José A. Varela[c] and Elson Longo[d]



Fluid Phase Equilibria 499 (2019) 112231

Contents lists available at ScienceDirect

Fluid Phase Equilibria

journal homepage: www.elsevier.com/locate/fluid

Distinct self-assembly aggregation patters of nanorods with decorated ends: A simple model study

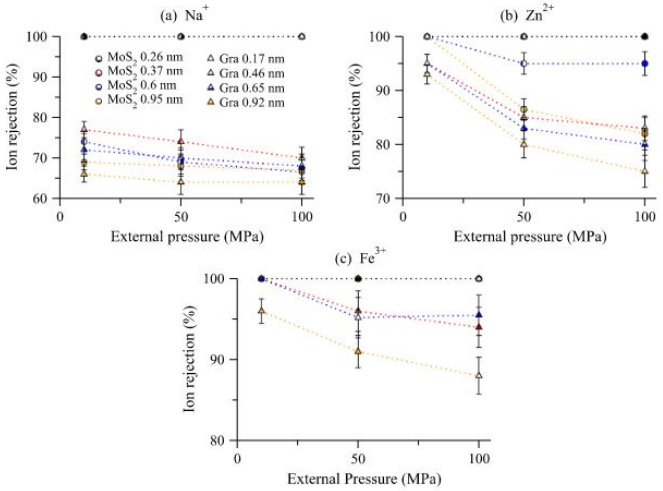
José Rafael Bordin

Da Ciência Básica pra Aplicada

Desastre da Samarco - Rio Doce

Desastre da Vale - Rio Paraopeba

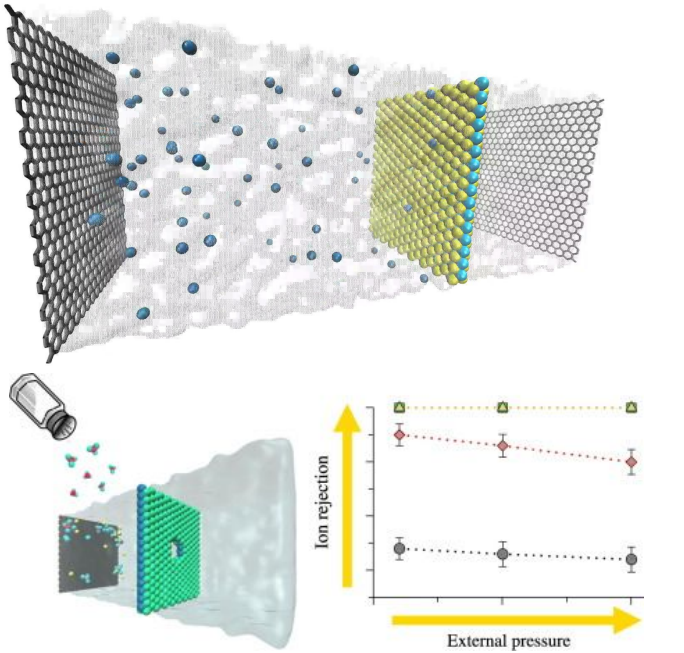
Nanofluídica



THE JOURNAL OF CHEMICAL PHYSICS **148**, 222804 (2018)

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

Mateus Henrique Köhler,[1,a)] José Rafael Bordin,[2,b)] and Marcia C. Barbosa[1]



Journal of Molecular Liquids 277 (2019) 516–521

Contents lists available at ScienceDirect

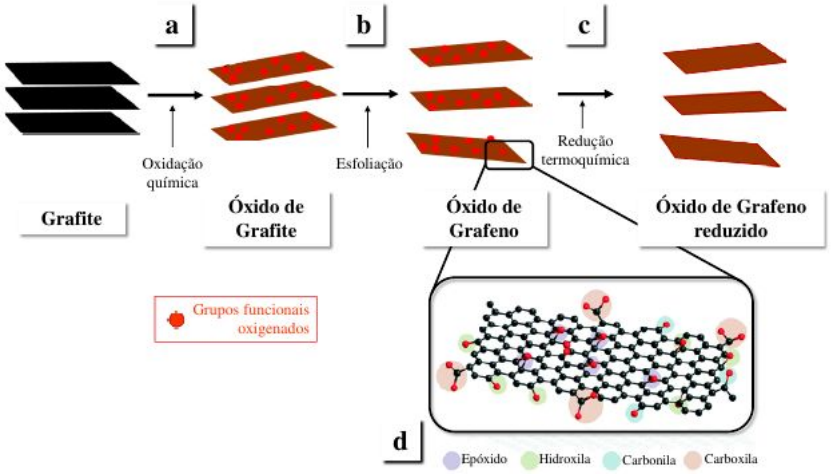
Journal of Molecular Liquids

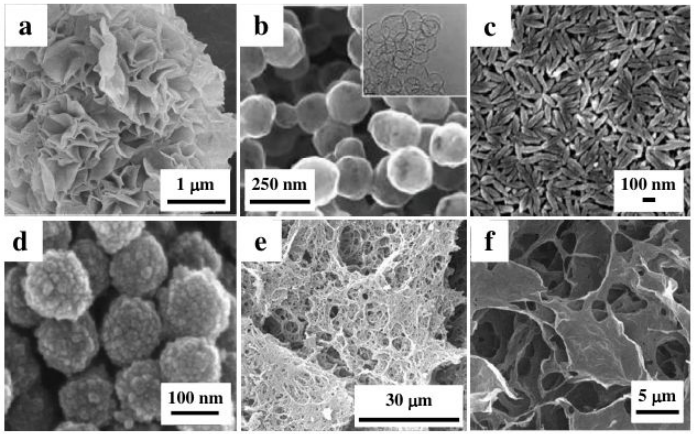
journal homepage: www.elsevier.com/locate/molliq

Ion flocculation in water: From bulk to nanoporous membrane desalination

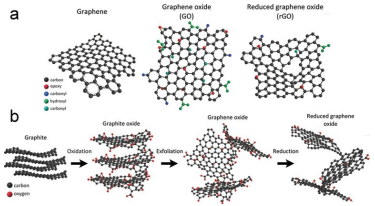
Mateus H. Köhler [a,b,*], José R. Bordin [c], Marcia C. Barbosa [b]

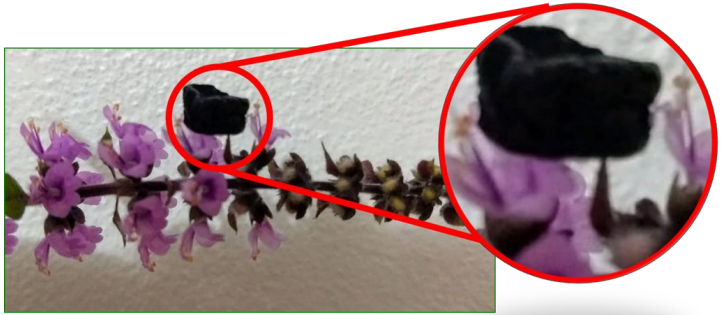
Nanomateriais





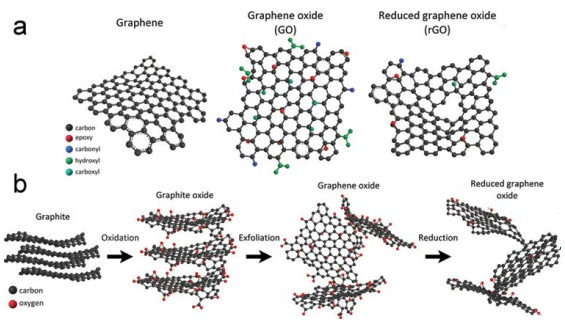
Nanomateriais

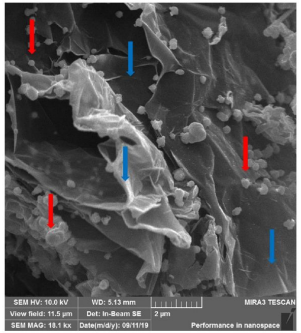


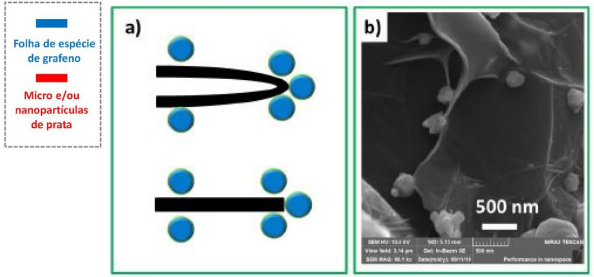


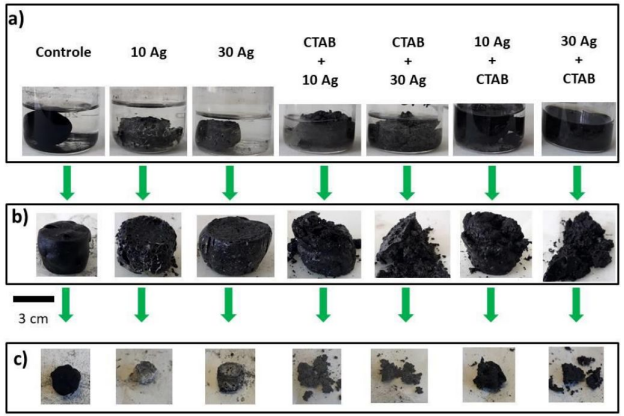
Processo de Obtenção de Estruturas Tridimensionais baseadas em Grafeno. C. F. Matos, M. B. Leão and JRB.
Patente: Privilégio de Inovação. Número do registro: BR10202001005, Instituição de registro: INPI – Instituto Nacional da Propriedade Industrial. Depósito: 20/05/2020

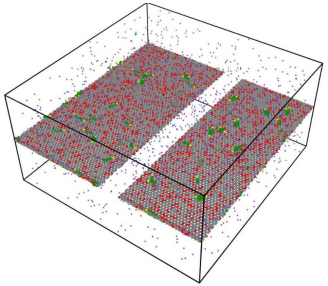
Nanomateriais

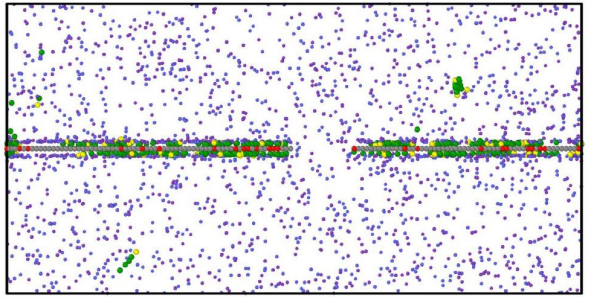






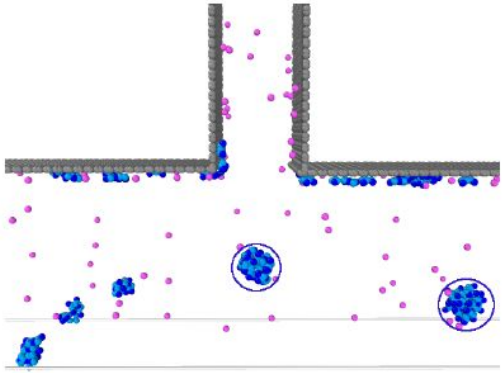


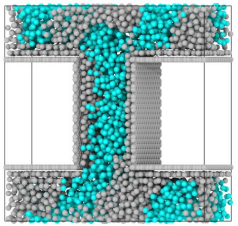


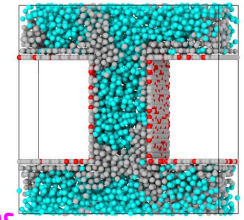


Processo de Obtenção de Macroestruturas Porosas de Grafeno e Partículas de Prata. C. F. Matos, P. C. C. da Rosa and JRB. Patente: Privilégio de Inovação. Número do registro: BR10202001803, Instituição de registro: INPI – Instituto Nacional da Propriedade Industrial. Depósito PCT: 03/09/2020

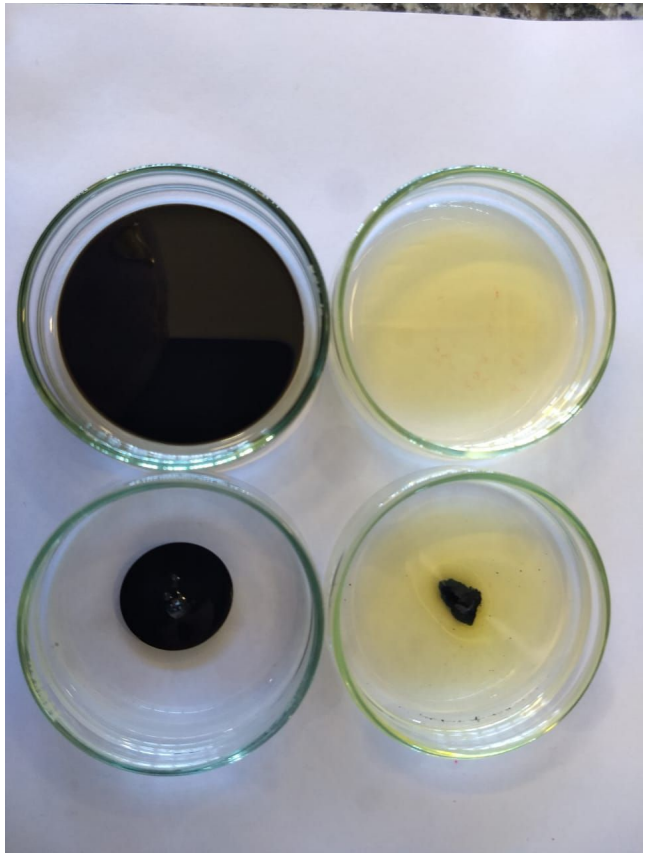
Nanomateriais & Nanofluídica







→ Metais Pesados
→ Óleo
→ Corantes
→ Fármacos
→ SarsCov2
→ Agrotóxicos
→ Hormônios
→ Cafeína



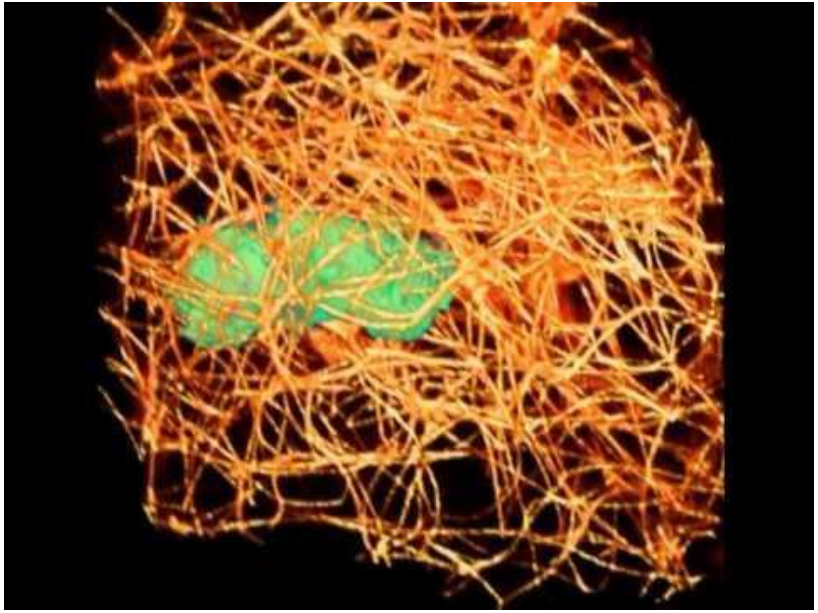
Até aqui...

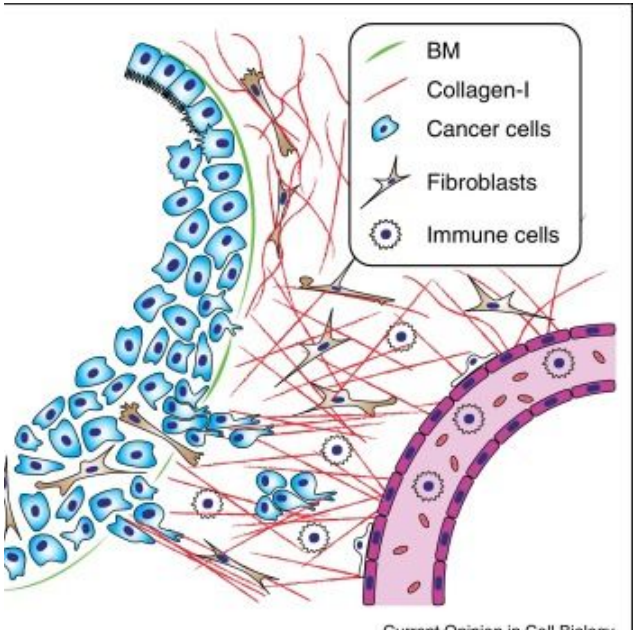
⟶ Como coisas andam em lugares muito apertados

⟶ Como coisas pequenas grudam e desgrudam

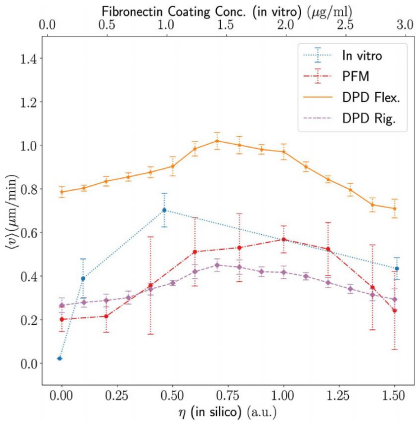
Classical Leap ⟶ Sistemas Biológicos

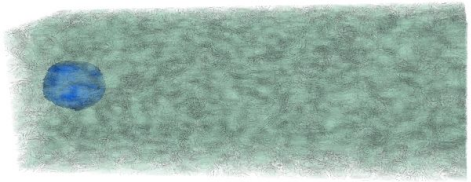
Difundindo em lugares apertados





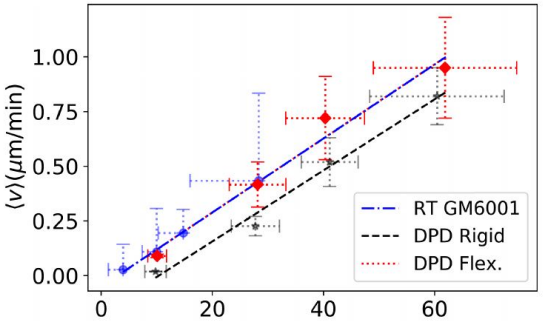
Células na Matriz Extra-Celular





Phase-Field Model

Dissipative Particle Dynamics Model

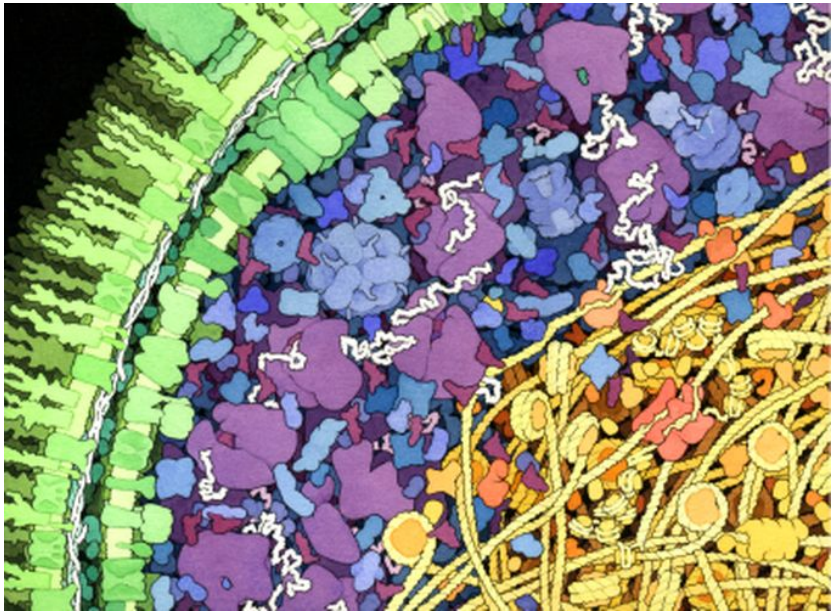


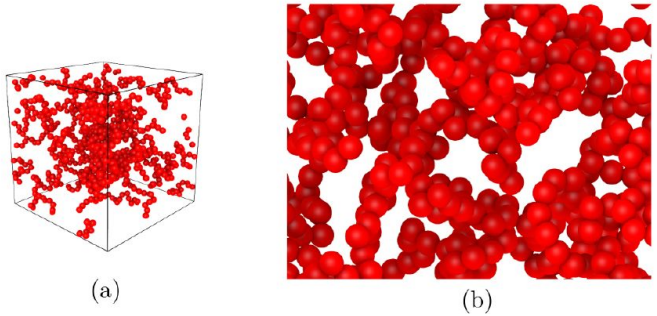
IOP Publishing — Journal of Physics: Condensed Matter
J. Phys.: Condens. Matter **32** (2020) 314001 (12pp) https://doi.org/10.1088/1361-648X/ab7c77

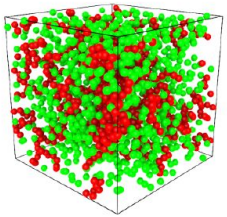
Adhesion modulates cell morphology and migration within dense fibrous networks

Maurício Moreira-Soares[1,4], Susana P Cunha[2], José Rafael Bordin[3] and Rui D M Travasso[1]

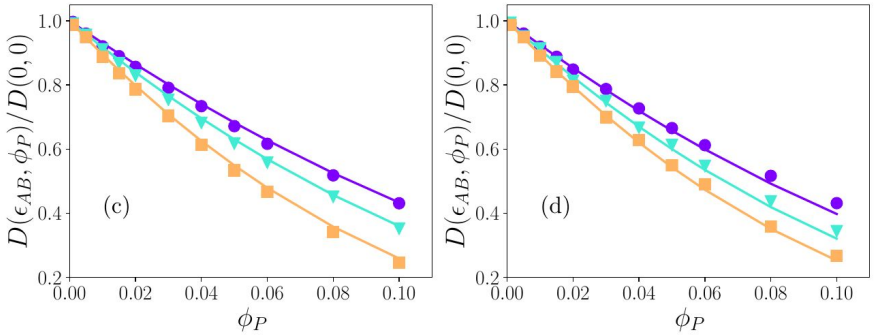
Macromolecular Crowding





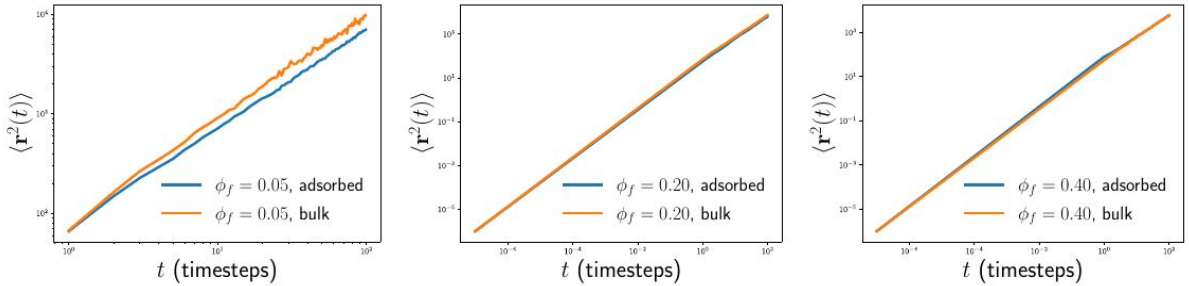


Macromolecular Crowding



Tortuosidade

$$\frac{D(\phi)}{D_0} \equiv \tau(\phi) = (1-\phi)^{\nu}[1-\lambda_p(\phi)]^{a+b\lambda_p(\phi)}$$



PHYSICAL REVIEW E
covering statistical, nonlinear, biological, and soft matter physics

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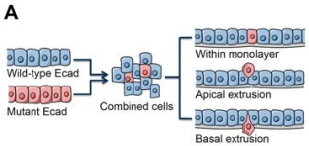
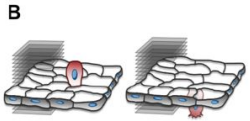
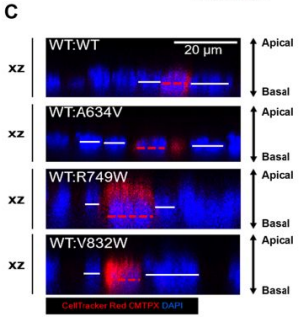
Tracer diffusion in crowded solutions of sticky polymers

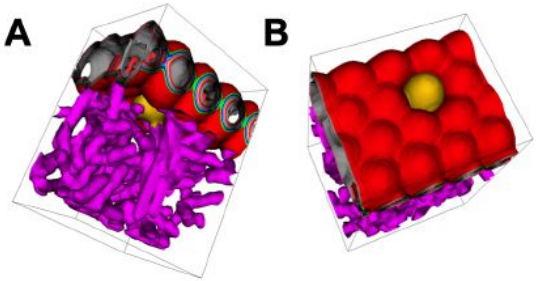
T. P. O. Nogueira, H. O. Frota, Francesco Piazza, and José Rafael Bordin
Phys. Rev. E **102**, 032618 – Published 29 September 2020

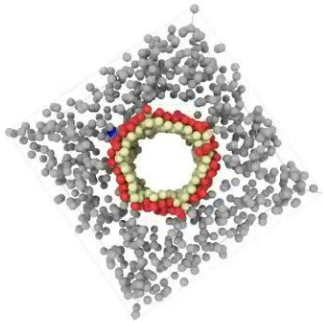
Câncer Gástrico Difuso

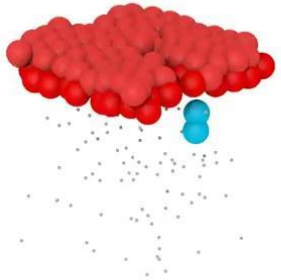


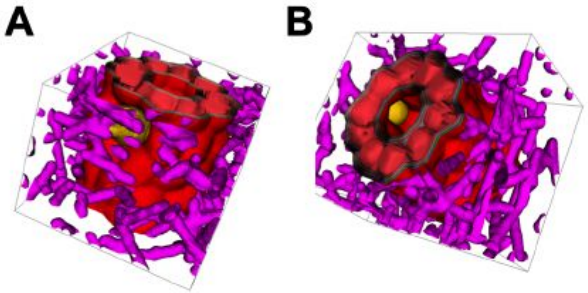












Stroma Invasion Driven by Loss of E-Cadherin Function - a mathematical modeling perspective on diffuse gastric cancer

Fátima Carneiro[d,e], Joana Figueiredo[d,e], João Carvalho[a], José Rafael Bordin[b], Maria Beatriz Dias[a], Maurício Moreira Soares[g], Pilar Guerrero[c], Raquel Seruca[d,e,f], Rui D.M. Travasso[a], Soraia Melo[d,e], and MAIS GENTE[c]

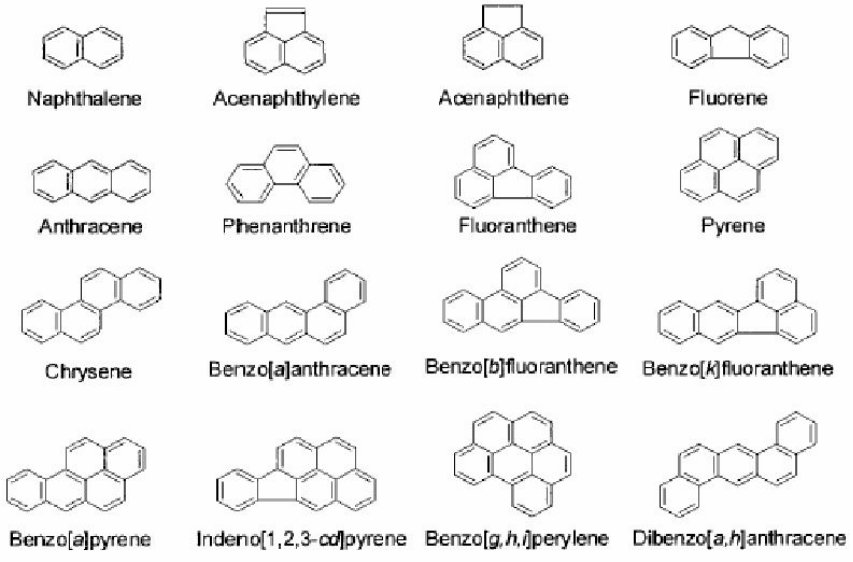
Até aqui...

⟶ Como coisas e biocoisas andam em lugares muito apertados

⟶ Como coisas e biocoisas grudam e desgrudam

Quantum Leap ⟶ Como coisas grudam no espaço!

PAHs

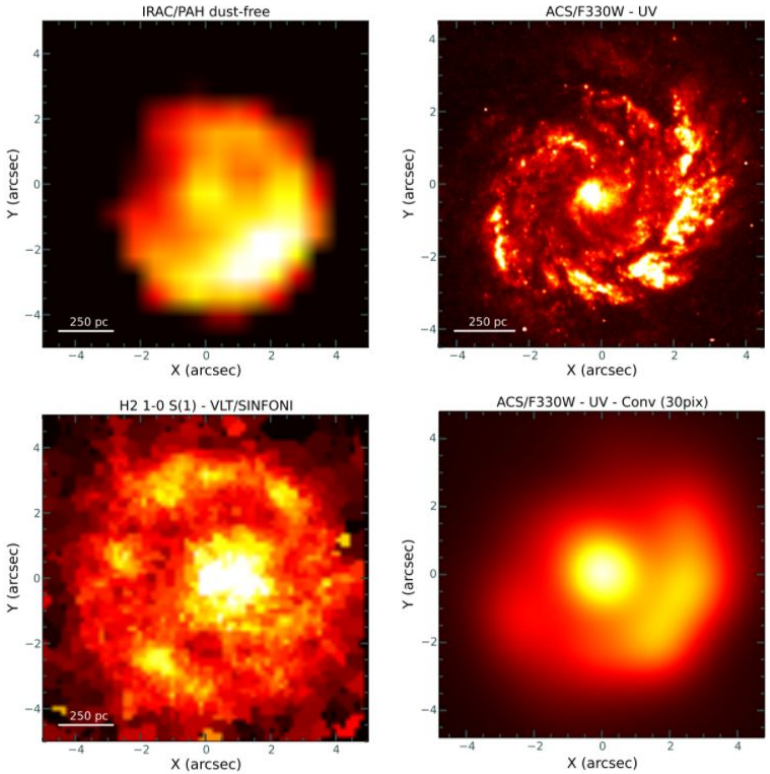


Os Hidrocarbonetos Aromáticos Policíclicos (PAHs) constituem uma família de compostos caracterizada por possuírem 2 ou mais anéis aromáticos condensados. Wikipédia

→ Material pré-biótico em condições extremas

Astroquímica Pré-biótica e formação de moléculas de interesse para a Astrobiologia

PAHs no centro de galáxias ativas

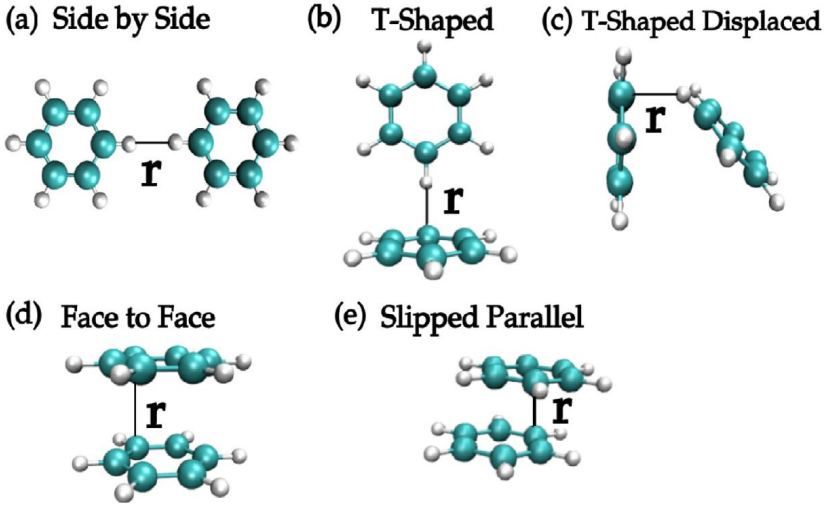


Topo-esquerda é uma imagem de PAH observada com o telescópio Spitzer. Topo-direita é uma imagem no UV observada com o telescópio Hubble e o abaixo-direito é a mesma imagem com um filtro gaussiano para simular a resolução angular da imagem do Spizter. Abaixo-esquerda é a imagem da molécula de H2 observado com o telescópio VLT no infravermelho próximo. Norte está para cima e leste está para a esquerda.*

**Foi o que a Dinalva me disse*

Self-Assembly de Benzeno em Condições Extremas

→ Primeiro passo: um modelo simples de benzeno [Physica A **537** 122679 (2020).]



Self-Assembly de Benzeno em Condições Extremas

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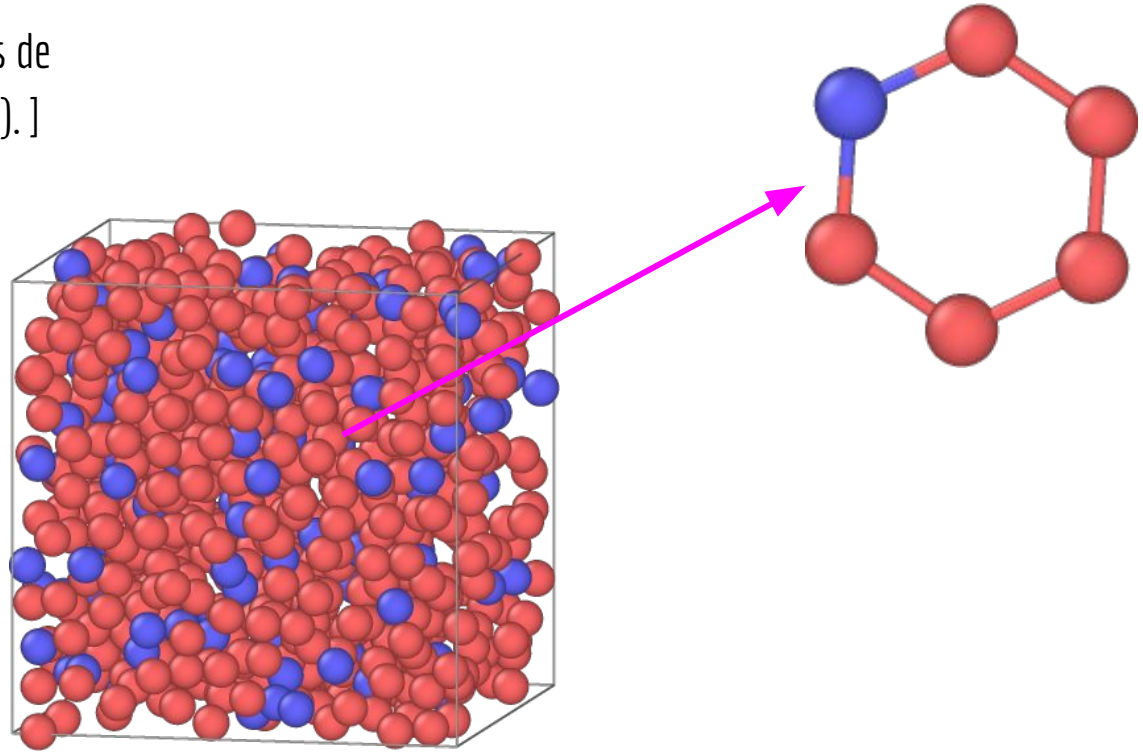
→ Segundo passo: colocar pra rodar



Self-Assembly de Benzeno em Condições Extremas

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⟶ Terceiro passo: construir o ferramental necessário para a análise dos dados e trajetórias (em progresso)

Self-Assembly de Benzeno em Condições Extremas

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→ Segundo passo: colocar pra rodar

→ Terceiro passo: construir o ferramental necessário para a análise dos dados e trajetórias (em progresso)

→ Quarto passo: incluir reações químicas

Agradecimentos

CAPES CNPq FAPERGS

Contato:

jrbordin@ufpel.edu.br

wp.ufpel.edu.br/bordin

@bordinLab