Multiscale atomistic simulation of complex materials for energy and infrastructure applications

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BR PETROBRAS

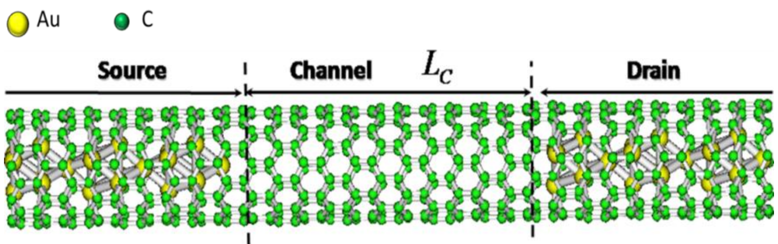
Nanopetro Research Group

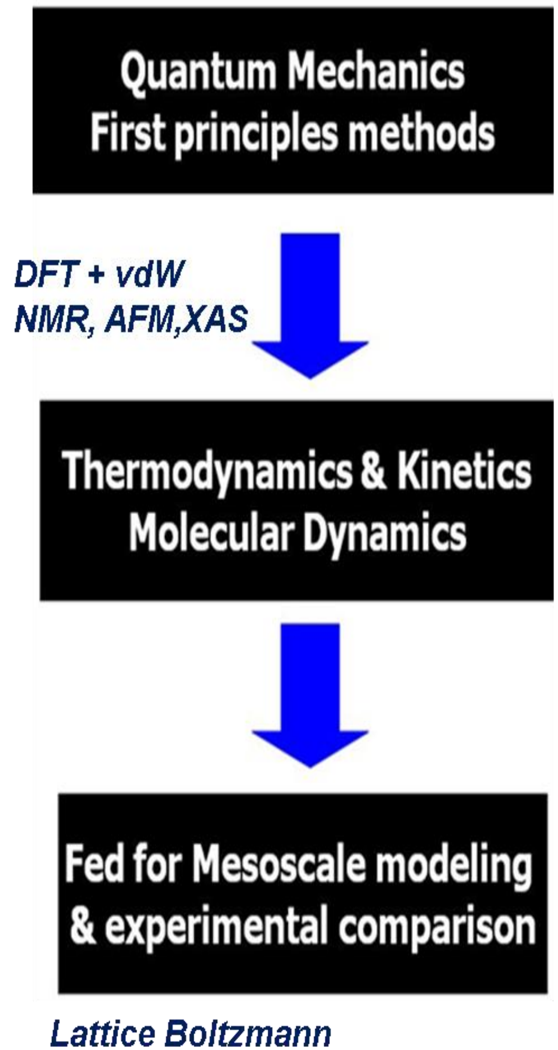
Goal: connect atomistic scale properties of materials to approach Brazil´s innovation industry challenges

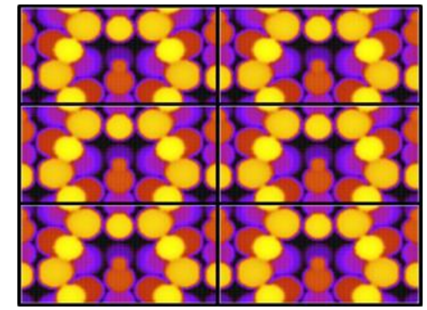
Highlights of our USP-Rice use:

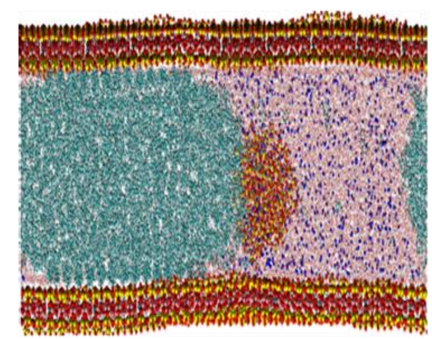
a) Oil & Gas
b) Infrastructure (cement and asphalt materials)
c) Energy storage and conversion

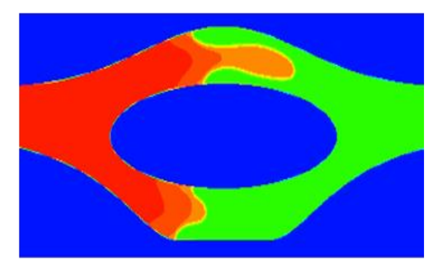
Computational modeling in materials design:
a multiscale approach



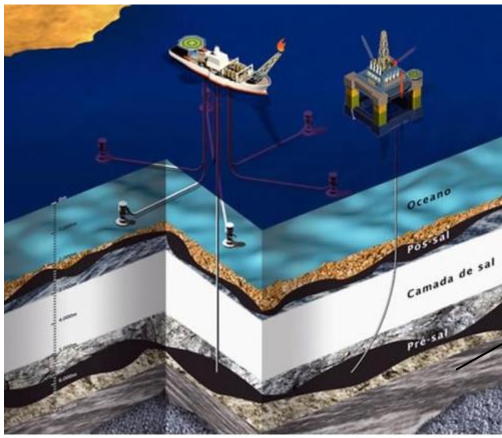


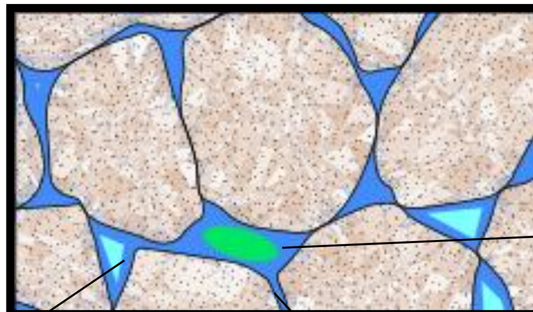




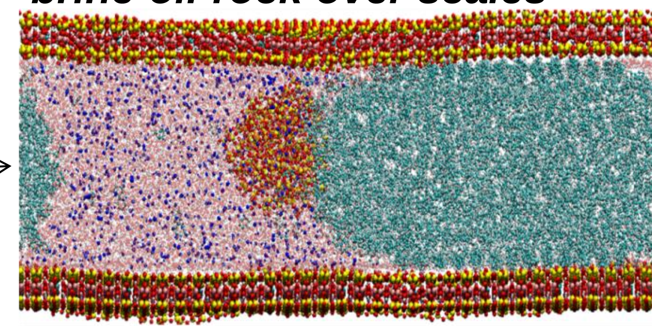


Nanoscience applied to O&G industry

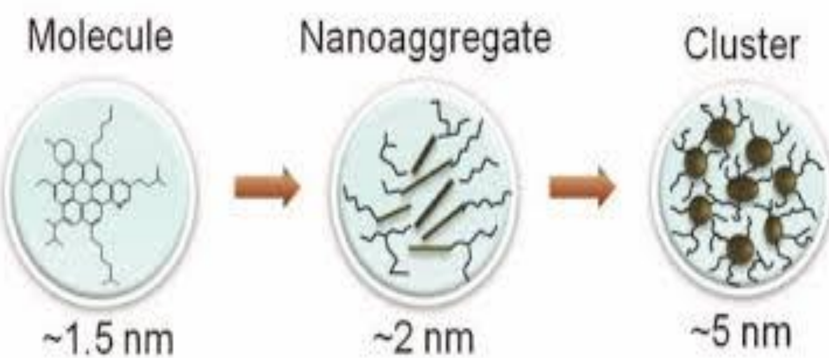




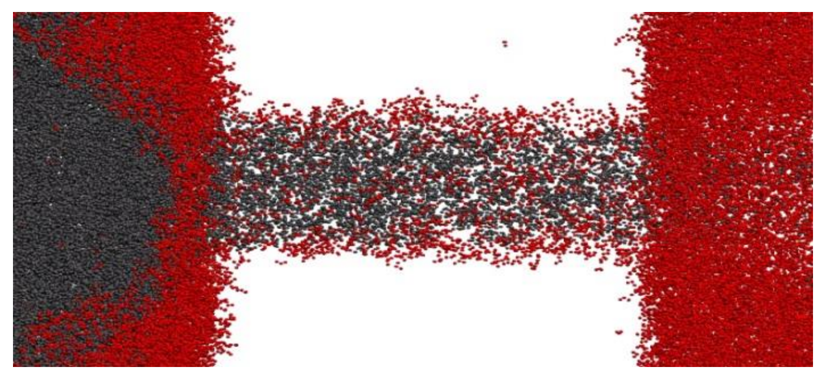
NANO-EOR - Surface driven flow: ***NPs at interfaces brine-oil-rock over scales***



ASPHALTENES
Aggregation of complex matter



NANO-IOR – Pressure driven flow
Fluid confinament,multiphasic fluids
Flow in NANO porous media

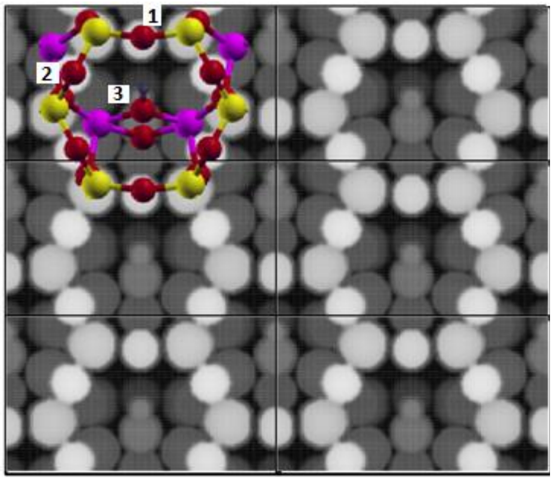


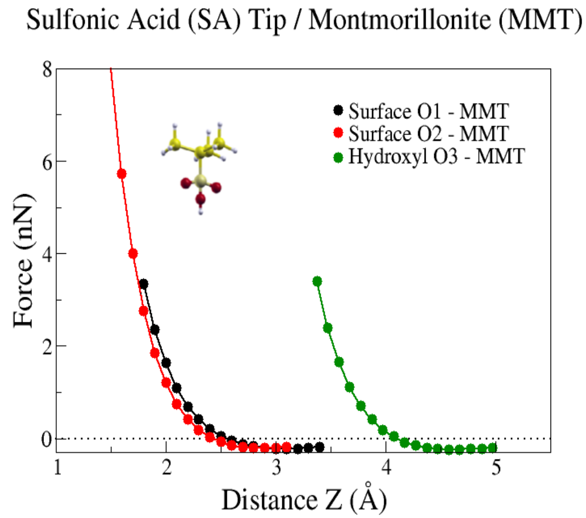
NANO-EOR

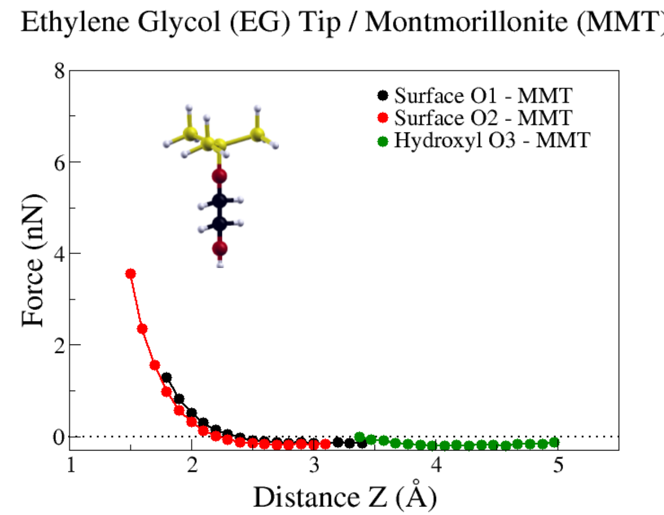
Surface driven flow

Alvim and Miranda, J. Phys. Chem. C, 120, 13503(2016)
Alvim and Miranda, Phys. Chem. Chem. Phys.,17, 4952 (2015)

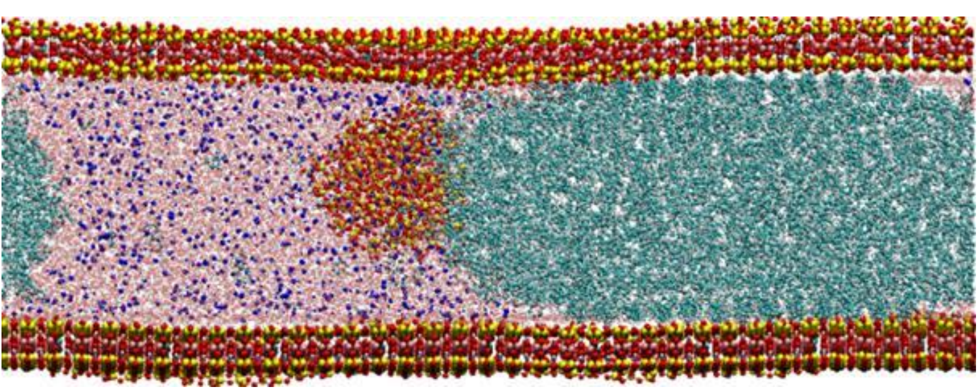
AFM Simulations Functional groups with Clay surface – DFT + vdW

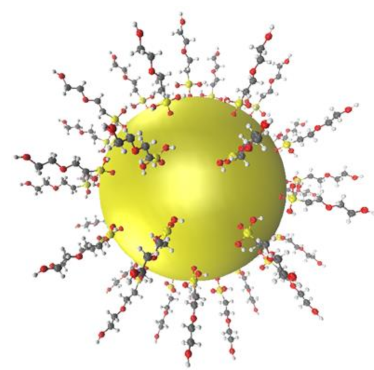


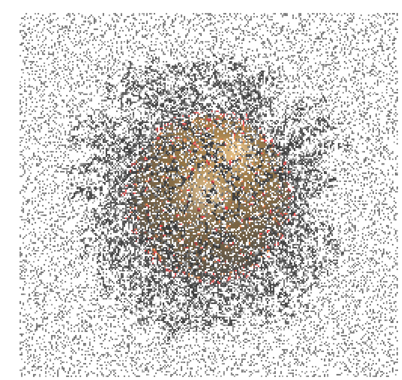




DIGITAL molecular OIL and ROCKS





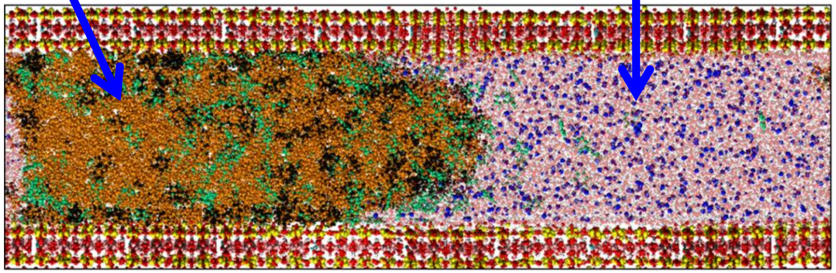


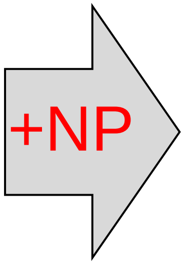
Fully atomistic to hybride models:
Larger NPs and magnetic systems

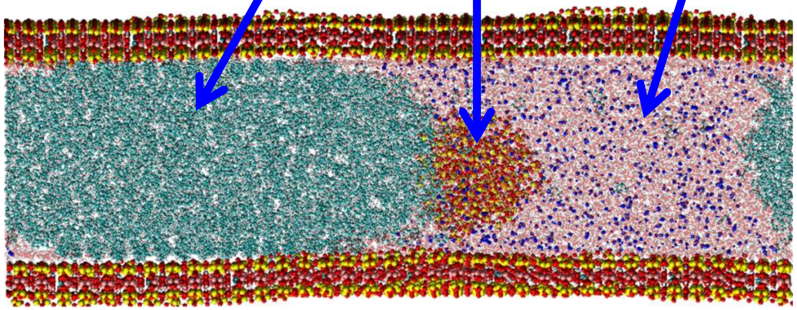
Going beyond MD

MD : nm ns
LBM : µm/mm µs/ms

T=300K – 400K and P=1 to 200atm





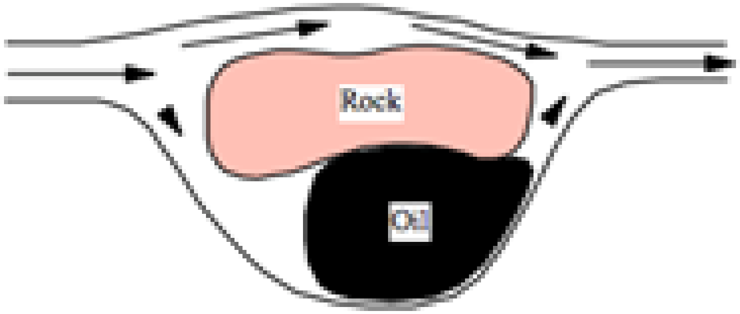


MD Physical properties

ρ_o=0.81 g/cm^3; ρ_b=0.96 g/cm^3;
η_o=3.62 mPa-s; η_b=0.79 mPa-s;
γ_{ob}=43 mN/m; θ_w= 28^o

ρ_o=0.81 g/cm^3; ρ_b=0.96 g/cm^3;
η_o=3.60 mPa-s; η_b=0.88 mPa-s;
γ_{ob}=38 mN/m; θ_w= 21^o

LBM parameters:
$G = 0.14$; G_w =-0.015;
$\tau_{oil} = 1.50$; τ_{brine}= 0.70

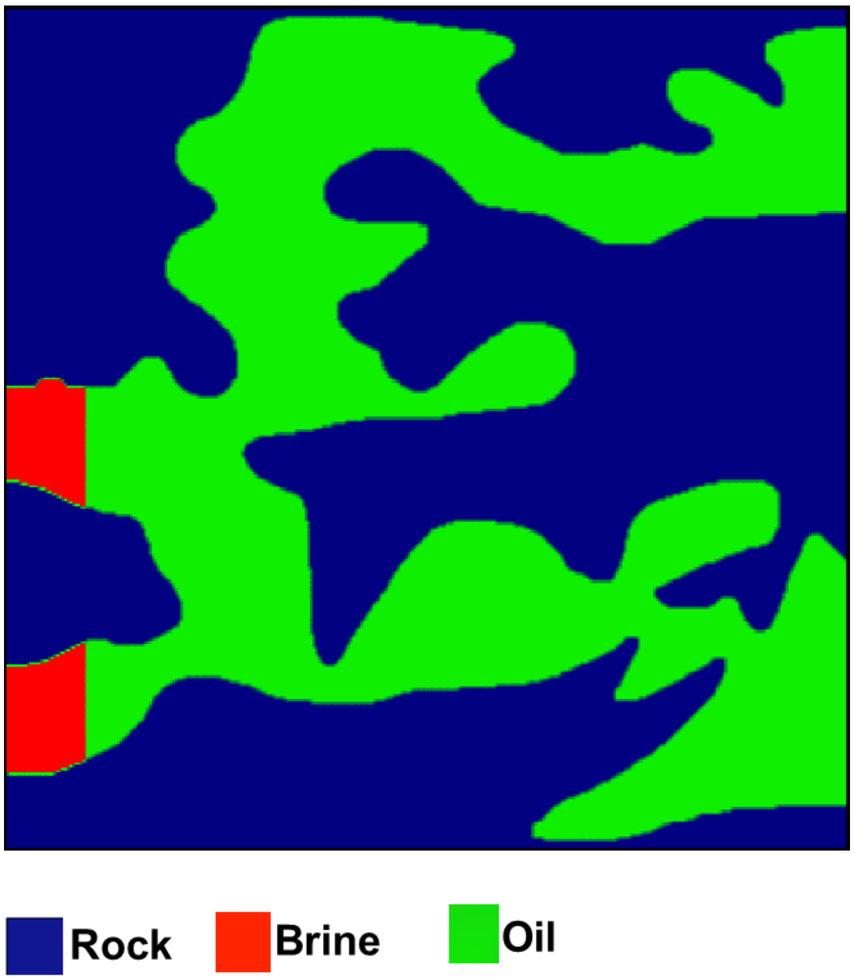


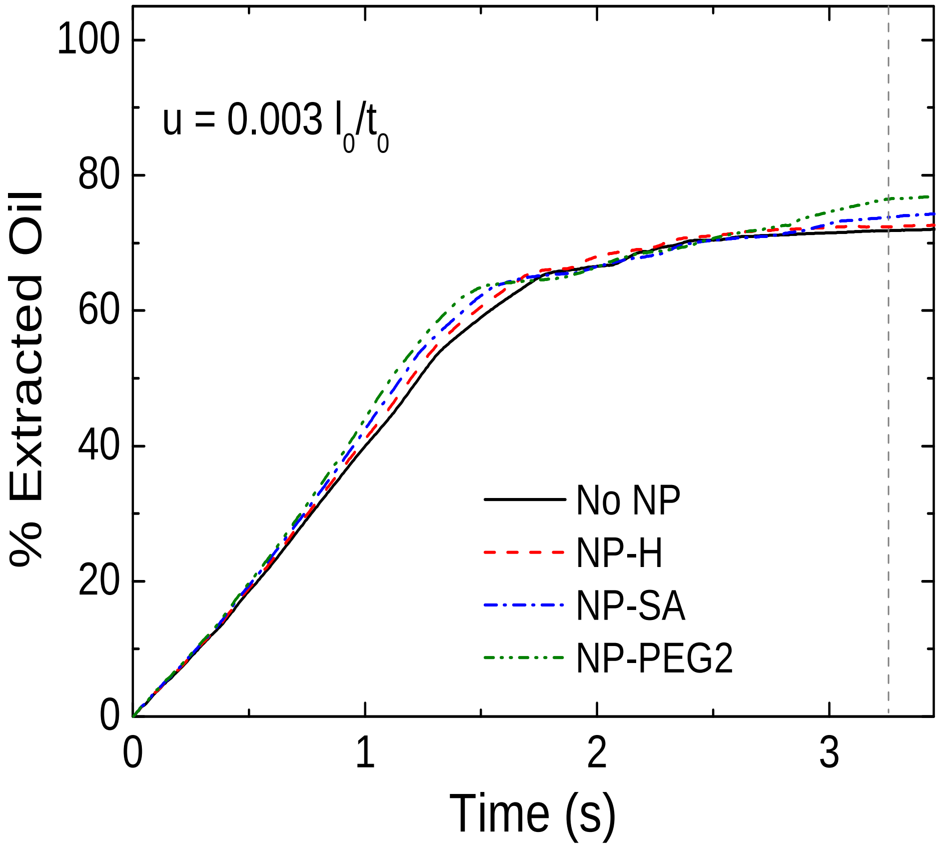
$G = 0.15$; G_w =-0.02;
$\tau_{oil} = 1.50$; τ_{brine} = 0.75

Exploring Oil Extraction by Nanofluids in Clay Coated Pore Network Models

Oil displacement by Brine+NP-PEG2: First Injection

$C_a = 1.2 \times 10^{-2}$

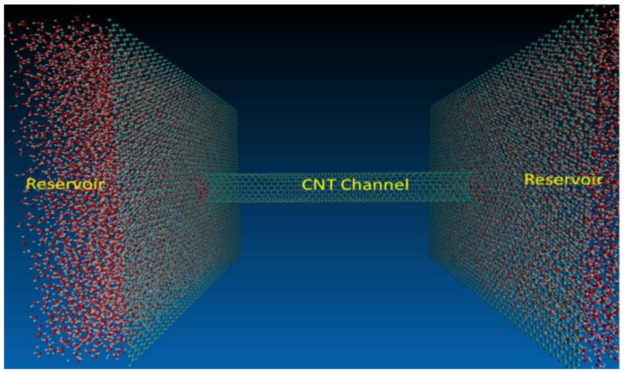


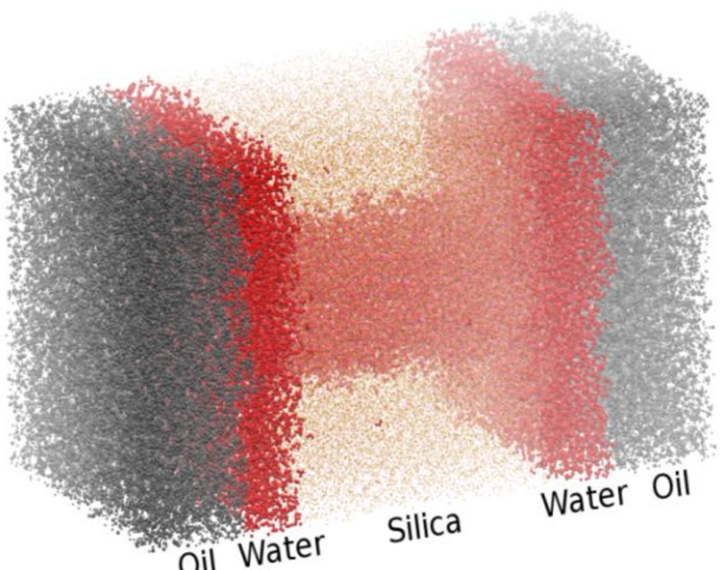


In collaboration with Sylvia Multisya, A. Kirch
J. M. de Almeida, V. M. Sanchez.

NANO-IOR: pressure driven flow

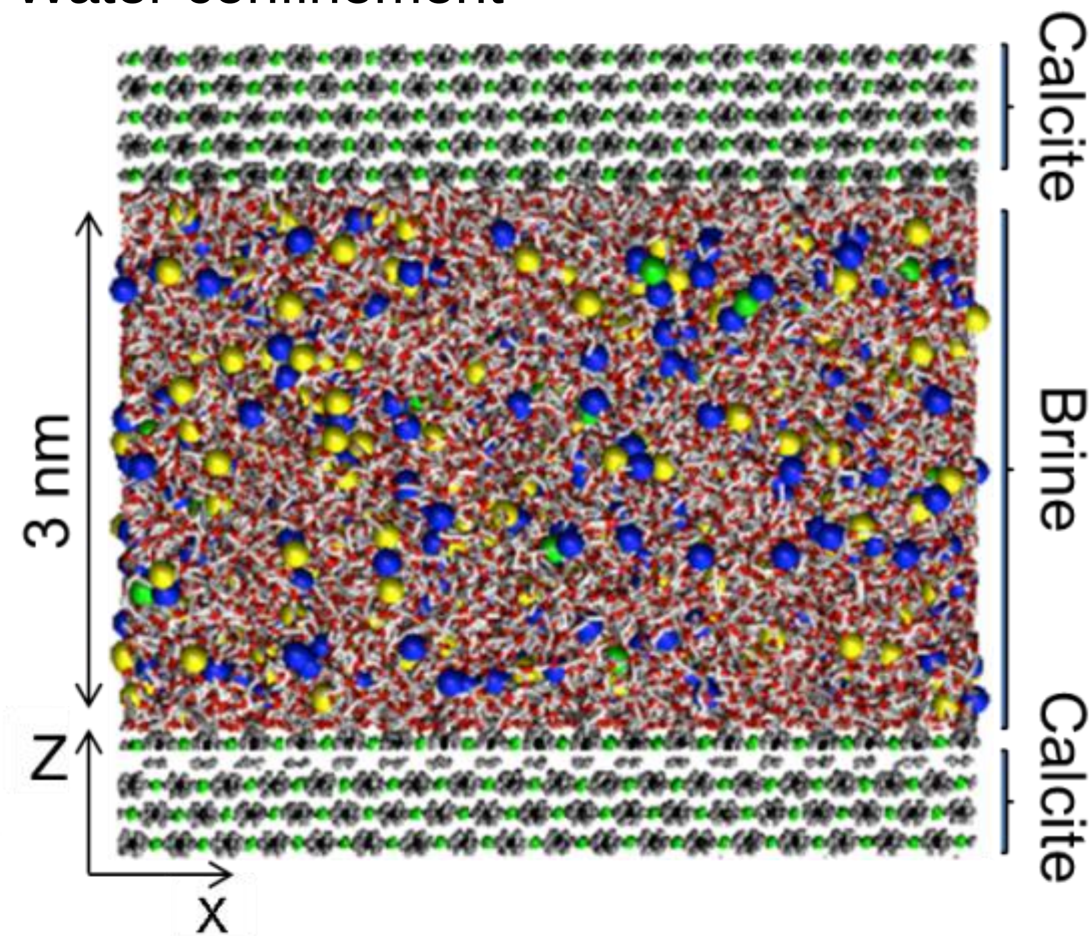
Nanofluidics





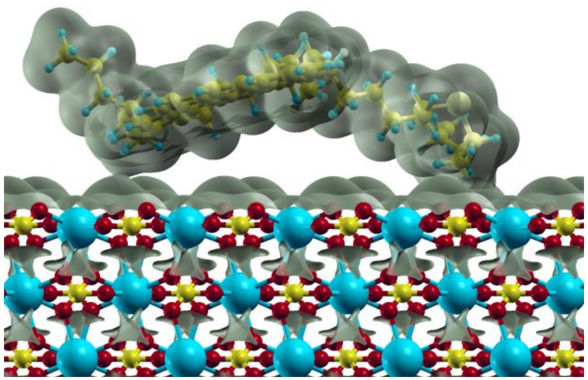
Almeida and Miranda
Scientific Reports (2016)

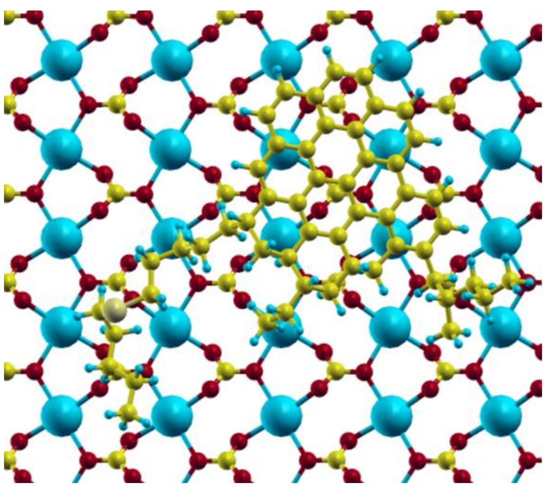
Water confinement



- SMART WATER – Low salt EOR “Água esperta”
- Structural properties of water/brine in calcite pores

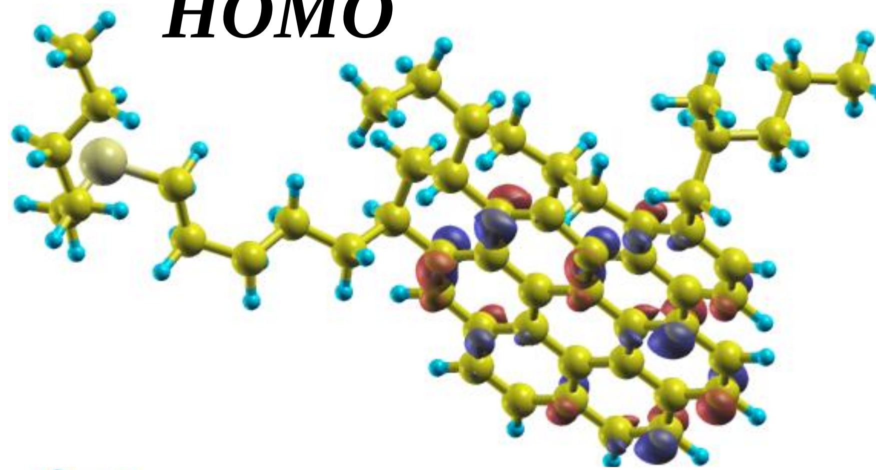
Asphaltenes adsorption on carbonates, silicates and stainless steel



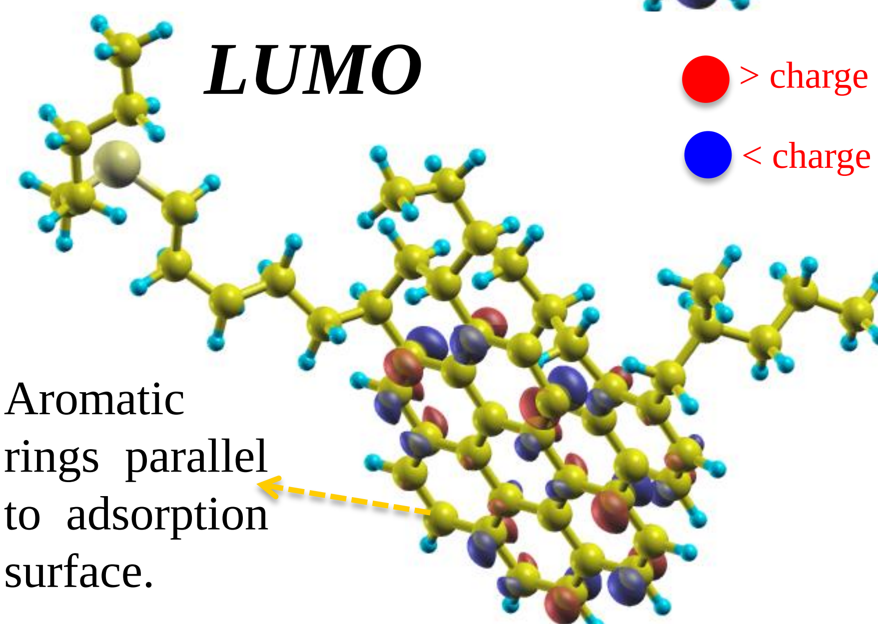


ΔE^{ads}= -56.20 kJ/mol (-0.58 eV)

HOMO



LUMO



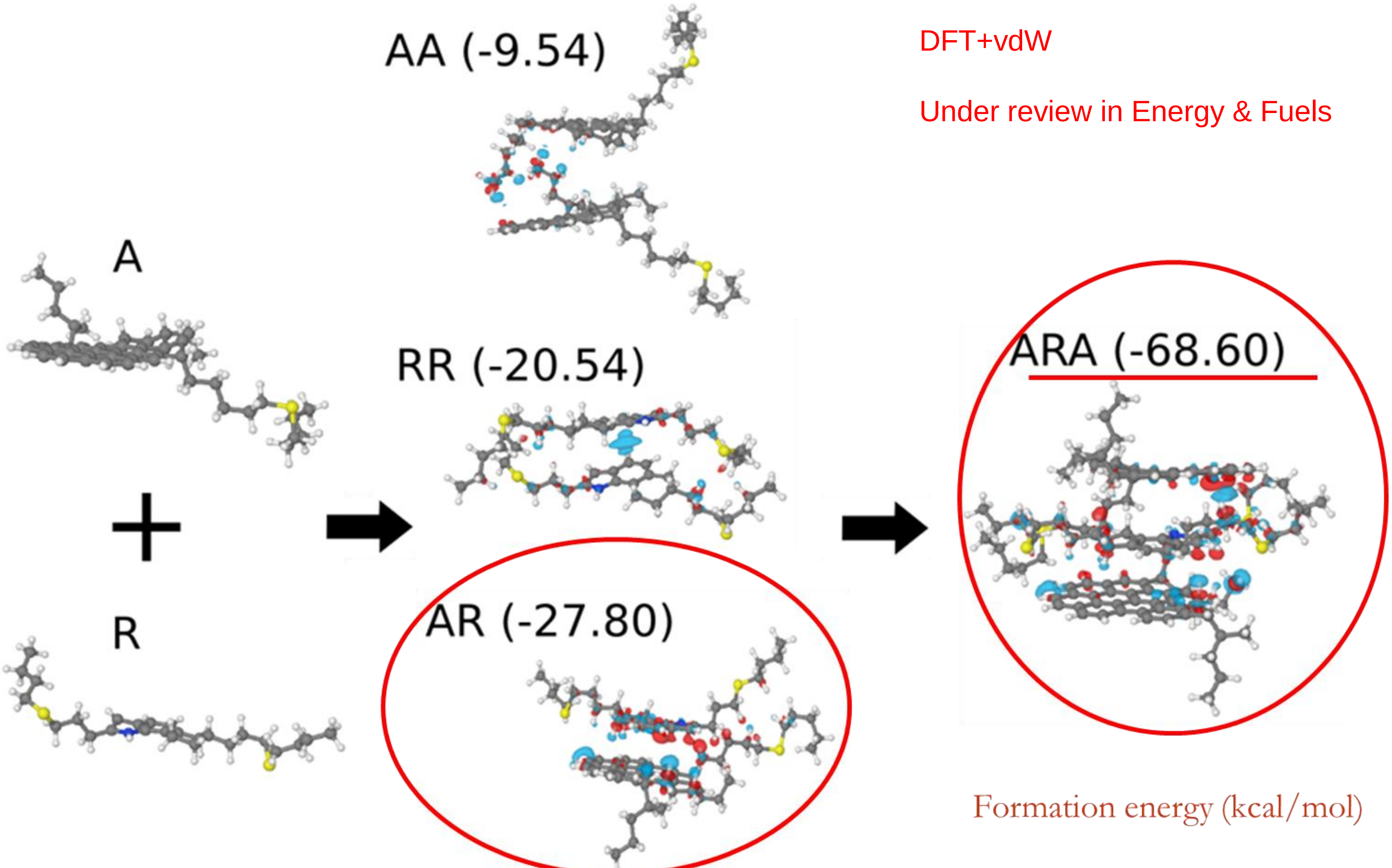
Aromatic rings parallel to adsorption surface.

In collaboration with Raphael Alvim and Filipe. D. Lima

Asphaltene nanoaggregation

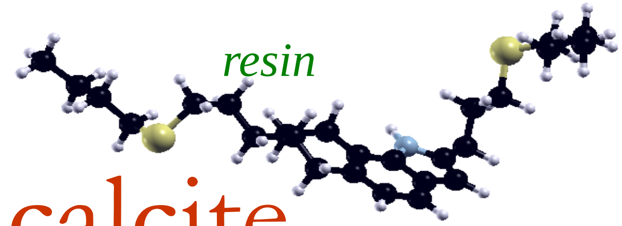
DFT+vdW

Under review in Energy & Fuels

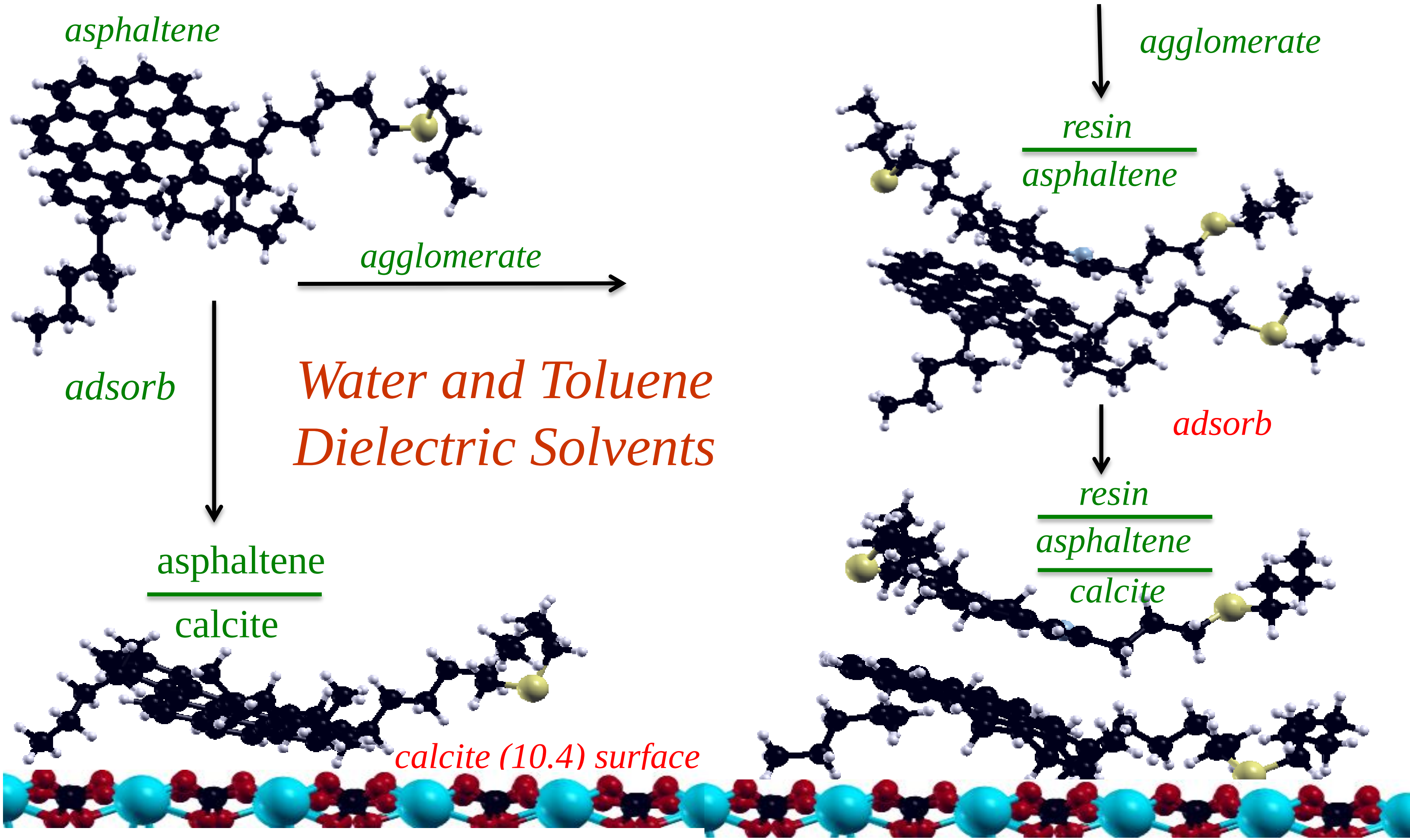


Formation energy (kcal/mol)

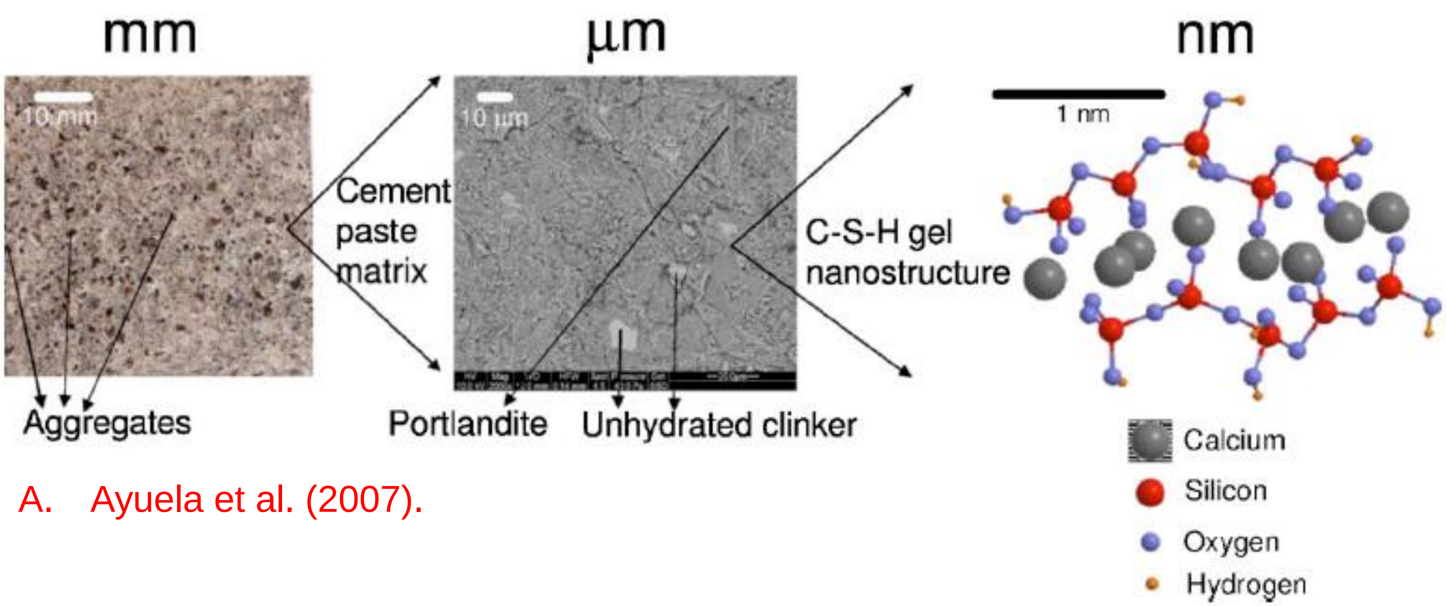
In collaboration with Raphael Alvim and Filipe. D. Lima
RSC Advances 2016



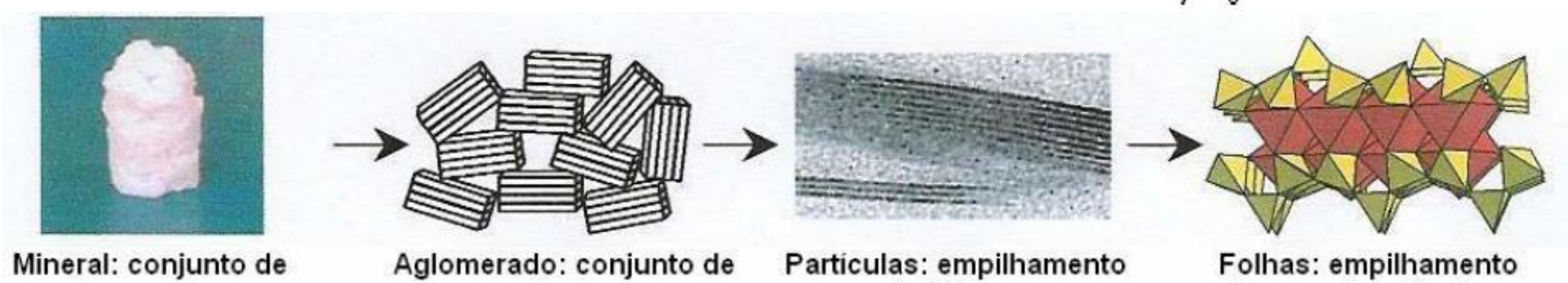
Asphaltene adsorption on calcite



Crossing scales in Cement based materials



A. Ayuela et al. (2007).

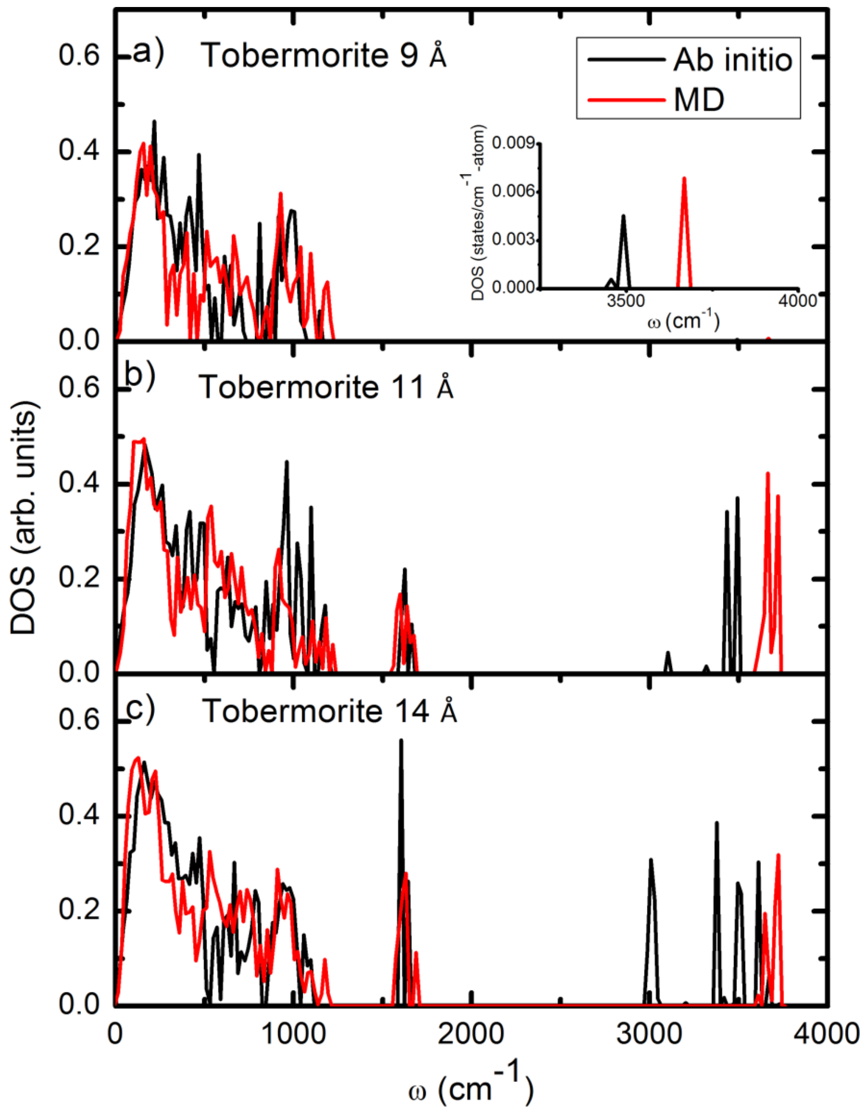


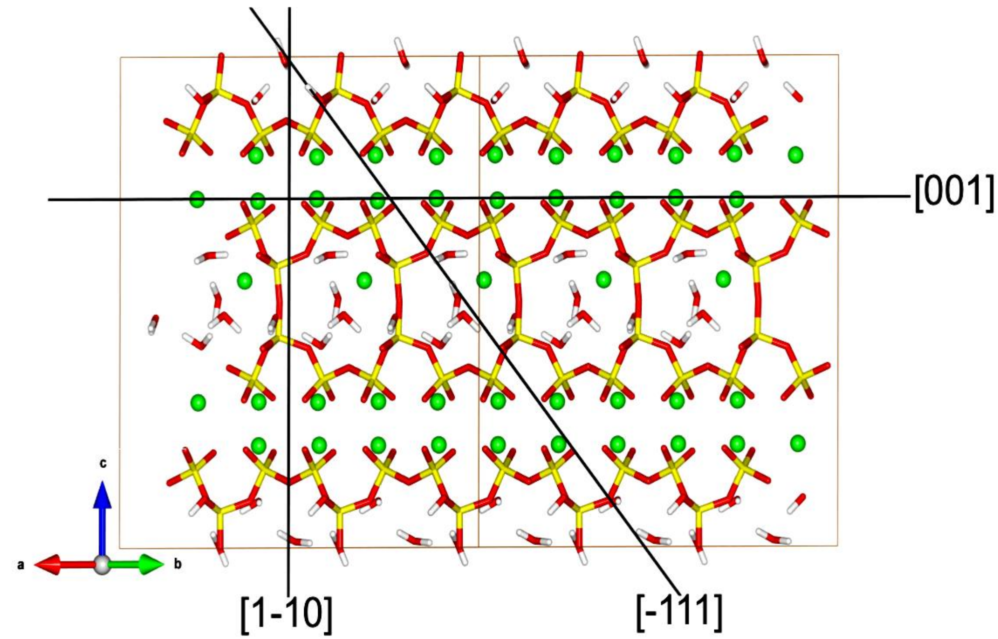
Calcium Silicate Hydrate – different length scales

10^{-2}m 10^{-6}m 10^{-8}m 10^{-9}m

MINET, J. PhD thesisFrança, 2003.

Cement: a first principles view

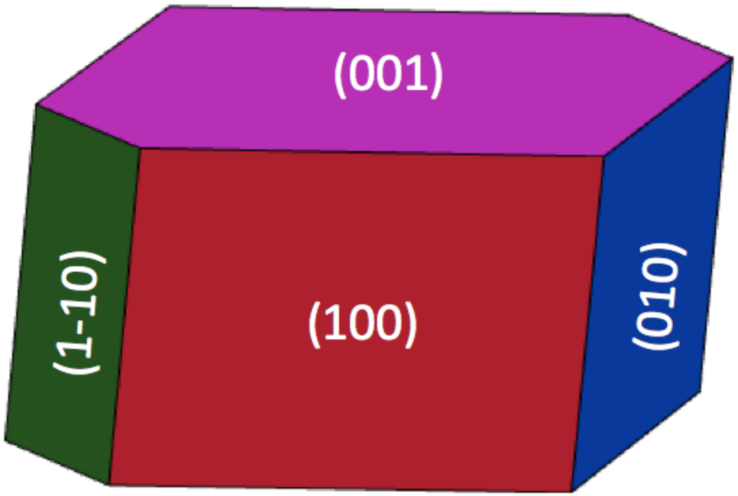




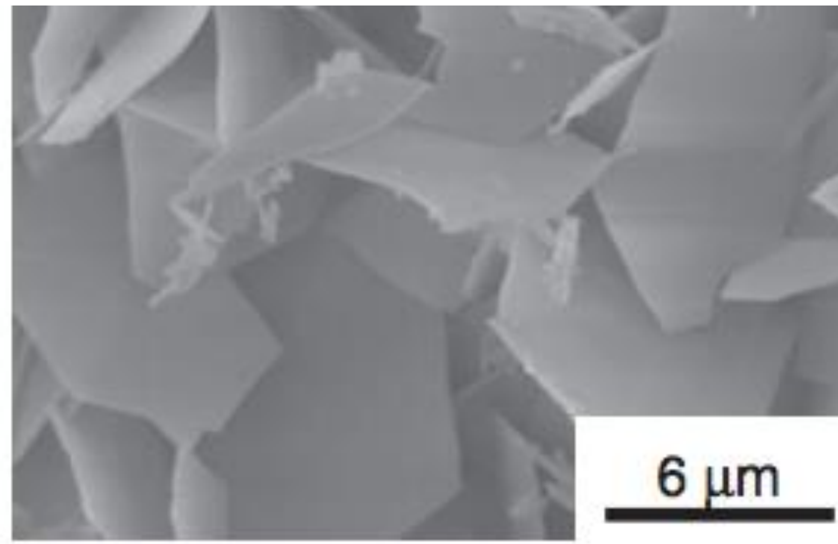
Surface termination	Surface energy (J/m^2)
(001)	0.46
(010)	0.88
(100)	0.69
$(1\bar{1}0)$	1.05
$(\bar{1}11)$	1.73
$(10\bar{1})$	1.22
$(0\bar{1}1)$	1.35

Cement: a first principles view

Morphology - Tobermorite 11 Å



Tobermorite 11 Å crystal based on surface energies

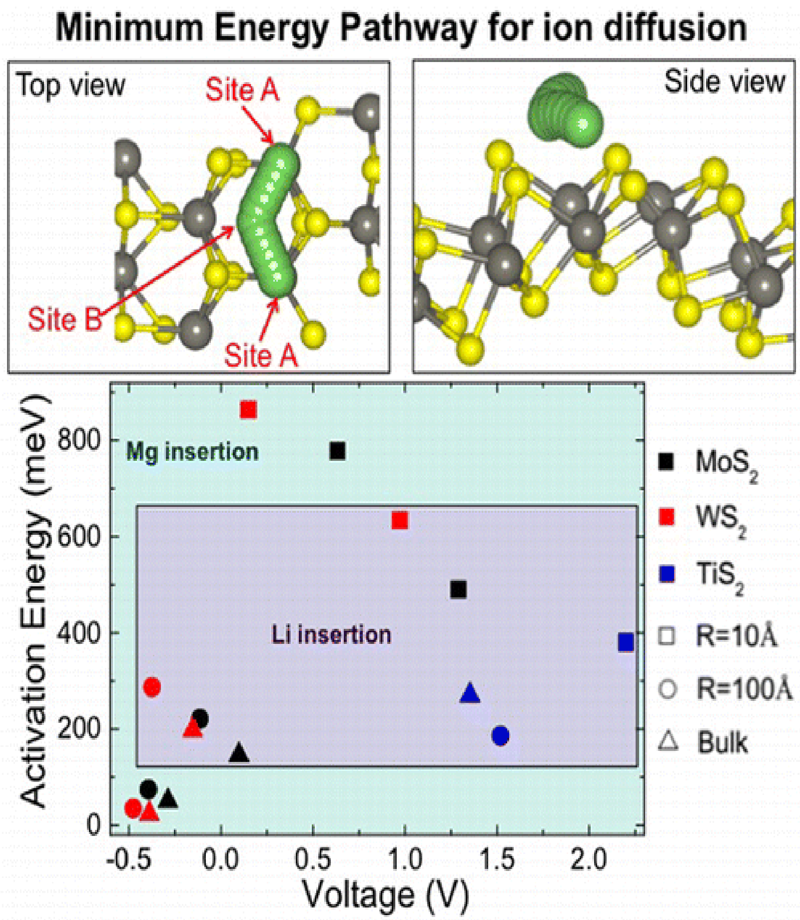


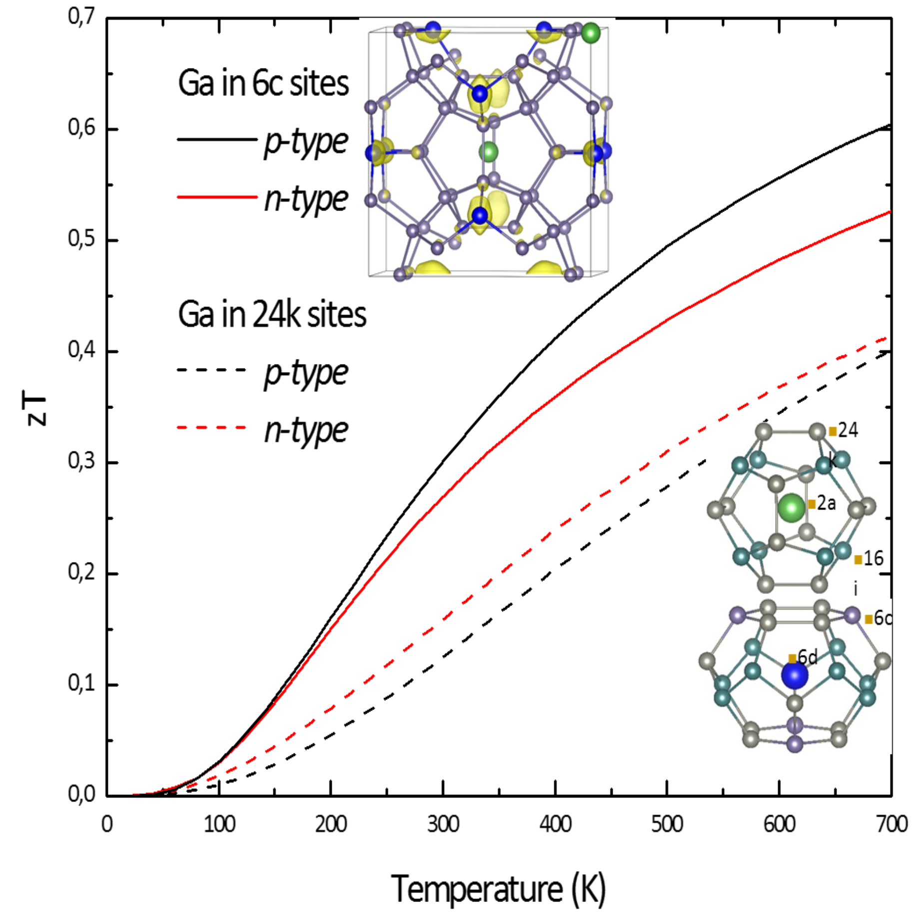
SEM image of hydrothermally synthesized tobermorite

- *Morphological importance is inversely proportional to the surface energy.*
- *The equilibrium morphology of Tobermorite 11 Å is pseudohexagonal.*

Journal of the Ceramic Society of Japan, 119(1389):375–377, 2011

Materials for energy storage and conversion: batteries and thermoelectrics



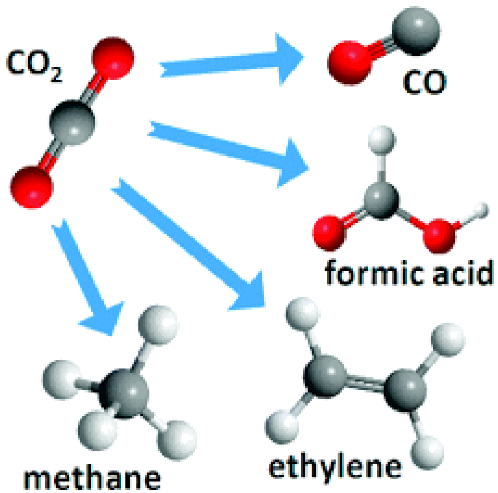


Comp. Materials Science (2016)
JPC_C (2015)

In collaboration with A.O. Pereira and A. Antonelli.

Materials for energy storage and conversion: Solar Fuels and Photocatalysts

Conversion of CO_2 into feedstock



$$CO_2(\text{solution}) \rightarrow CO_2(\text{ads}) \quad (1)$$

$$CO_2(\text{ads}) + e^- \rightarrow CO_2^{\bullet -}(\text{ads}) \quad (2)$$

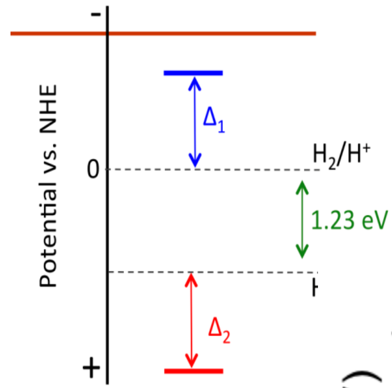
$$CO_2^{\bullet -}(\text{ads}) + HCO_3^- + e^- \rightarrow HCO_2^-(\text{ads}) + CO_3^{2-} \quad (3)$$

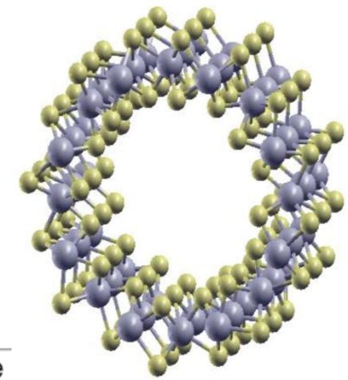
$$HCO_2^-(\text{ads}) \rightarrow HCO_2^-(\text{solution}) \quad (4)$$

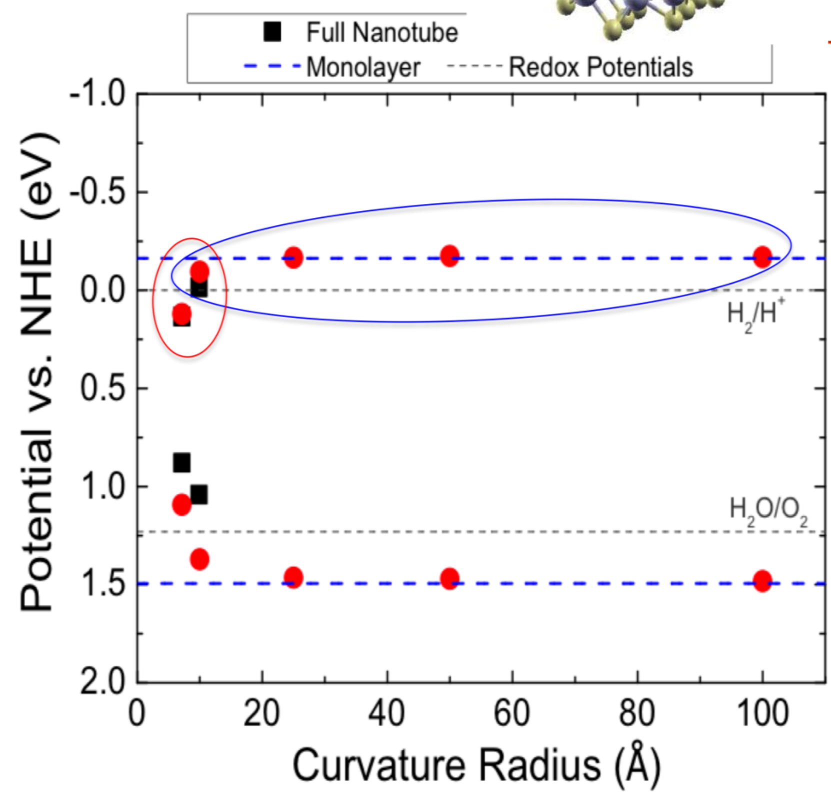
$$CO_3^{2-} + CO_2 + H_2O \rightarrow 2HCO_3^- \quad (5)$$

MRS meeting 2016

MoS_2 for water spliting







Summary (thanks to USP-Rice)

- Integrated multiscale approach (bottom-up and top-down)
- Understanding the underlying molecular mechanisms of phenomena at nanoscale
- Cost effective way to explore nanostructures under controlled, realistic and operational conditions.
- Materials design over a broad portfolio of energy and infrastructure technologies.