DEPARTMENT OF CHEMICAL & PROCESS ENGINEERING

University of Strathclyde Engineering

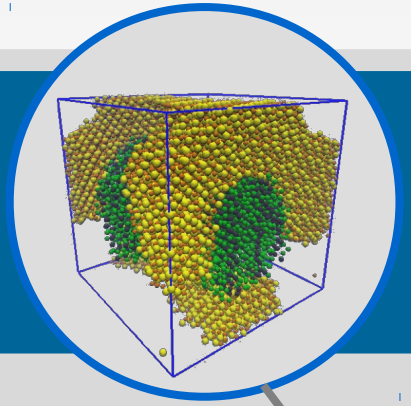
Computer-aided Design of Bio-inspired Nanoporous Silica Materials

By André Crescenzo

Miguel Jorge
Supervisor
Department of Chemical and Process Engineering

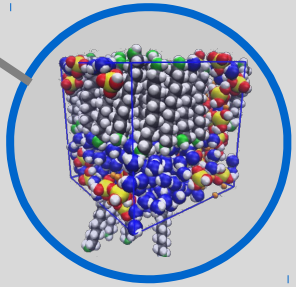
Alessia Centi
Supervisor
Department of Chemical and Process Engineering

Carlos F. Rangel
Supervisor
Department of Chemical and Process Engineering



MagiC

GROMACS FAST. FLEXIBLE. FREE.



Silica-surfactant materials

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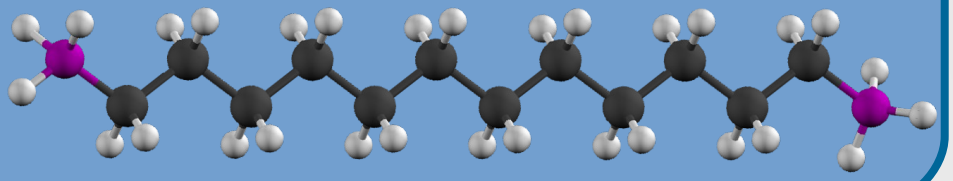
Highly Structured Materials

High Porosity
High Surface area

Generated by

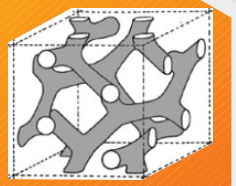
MSU-V

1,2-diaminododecane



Synthesis

MCM-50



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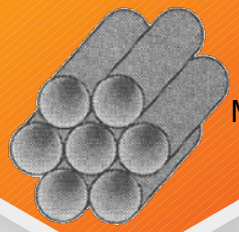
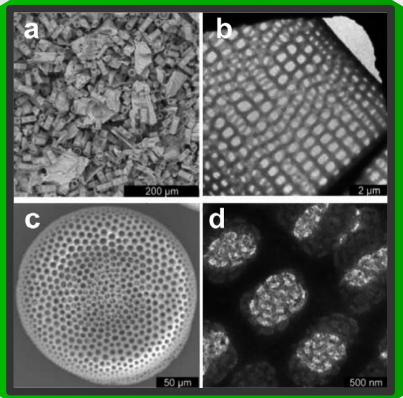


MCM-41

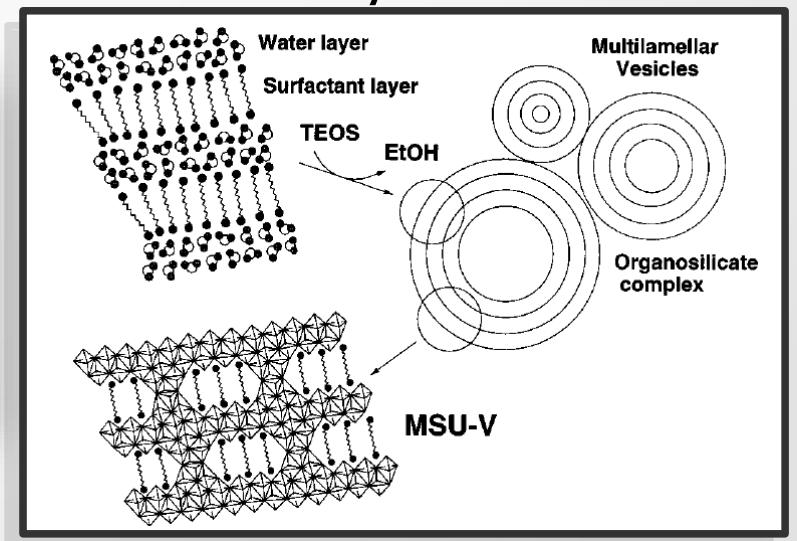
DOI:10.1039/C3CS60016E

Nature



DOI:10.1039/C0CC05648K

Self-Assembly structure



DOI:10.1021/ja970228v

Molecular simulation

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Molecular Dynamics

Newton's Law

$$m_i \frac{d^2 \vec{r}_i(t)}{dt^2} = \vec{F}_i(t)$$

"Leap-frog" Algorithm

$$\vec{r}_i(t + \Delta t) = \vec{r}_i(t) + \vec{v}_i(t + {}^{\Delta t}/_2)\Delta t$$

$$\vec{v}_i(t + {}^{\Delta t}/_2) = \vec{v}_i(t - {}^{\Delta t}/_2) + \frac{\vec{F}_i(t)}{m_i}\Delta t$$

Monte Carlo Simulations

Probability distribution function

$$\rho(\lambda) = \frac{\exp\left(-\frac{U(\lambda)}{kT}\right)}{\int_V \dots \int_V \exp\left(-\frac{U(\lambda)}{kT}\right) d\vec{r}_1\, d\vec{r}_2 \dots d\vec{r}_{\mathcal{N}}}$$

Metropolis Method

$$P_{1 \mapsto 2} = \begin{cases} 1 & for\ \frac{\rho(\lambda_2)}{\rho(\lambda_1)} \geqslant 1 \\ \frac{\rho(\lambda_2)}{\rho(\lambda_1)} & for\ \frac{\rho(\lambda_2)}{\rho(\lambda_1)} < 1 \end{cases}$$

Coarse-graining

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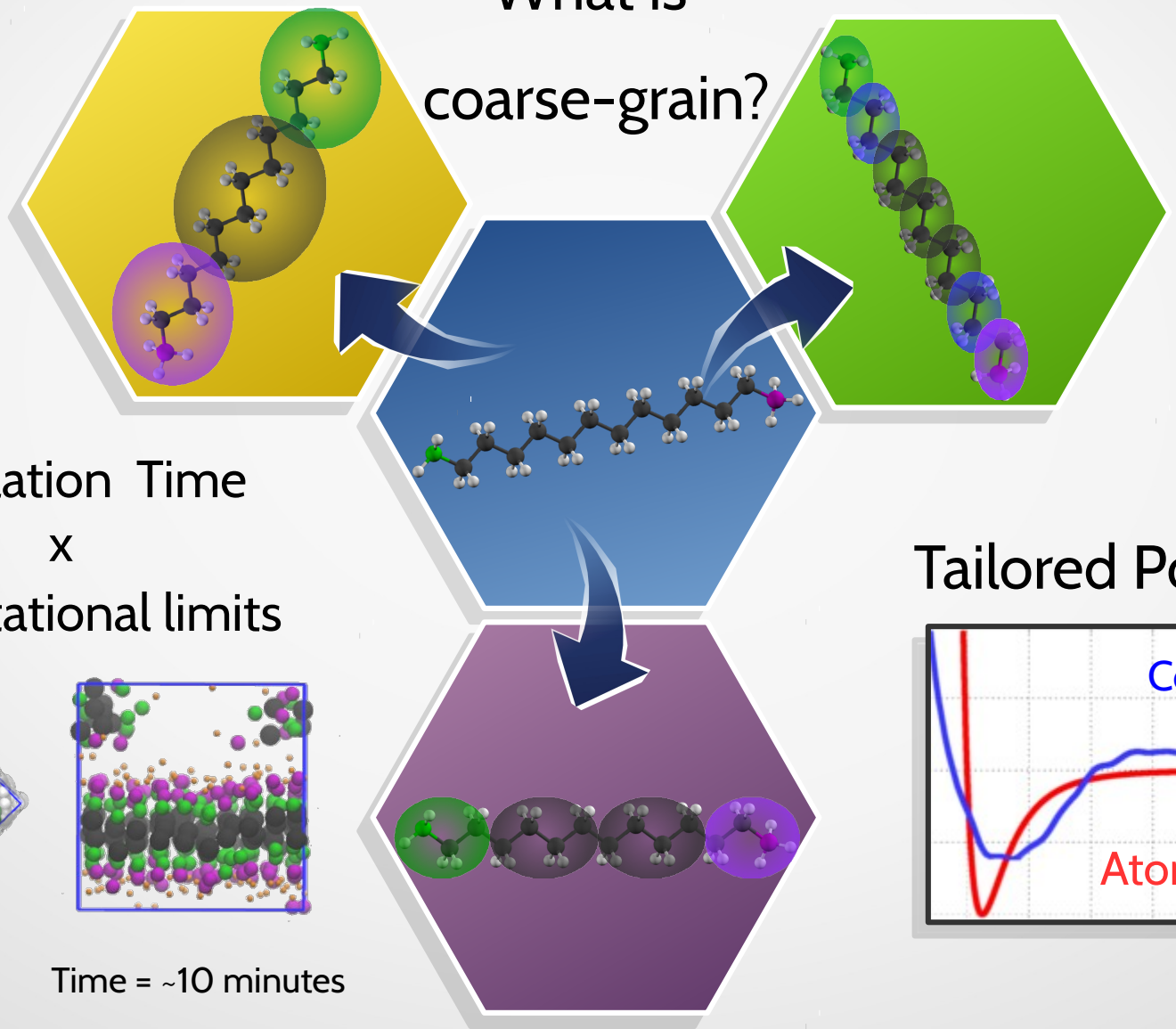
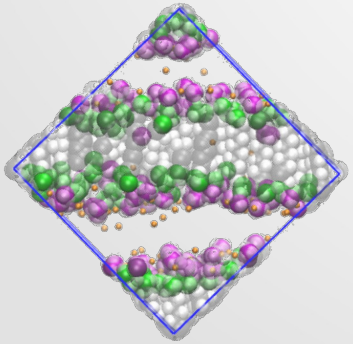
What is coarse-grain?



Simulation Time
x
Computational limits



Time = ~1,5 days

Time = ~10 minutes

Tailored Potentials

MagiC: a systematic method

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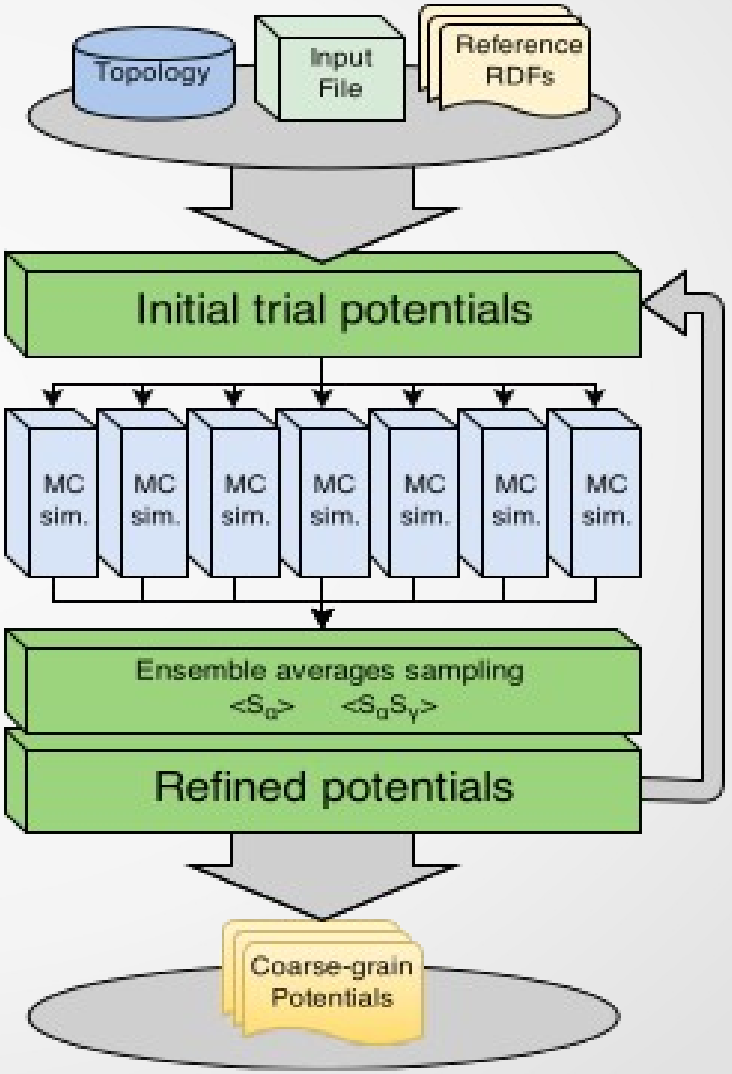
Boltzmann inversion

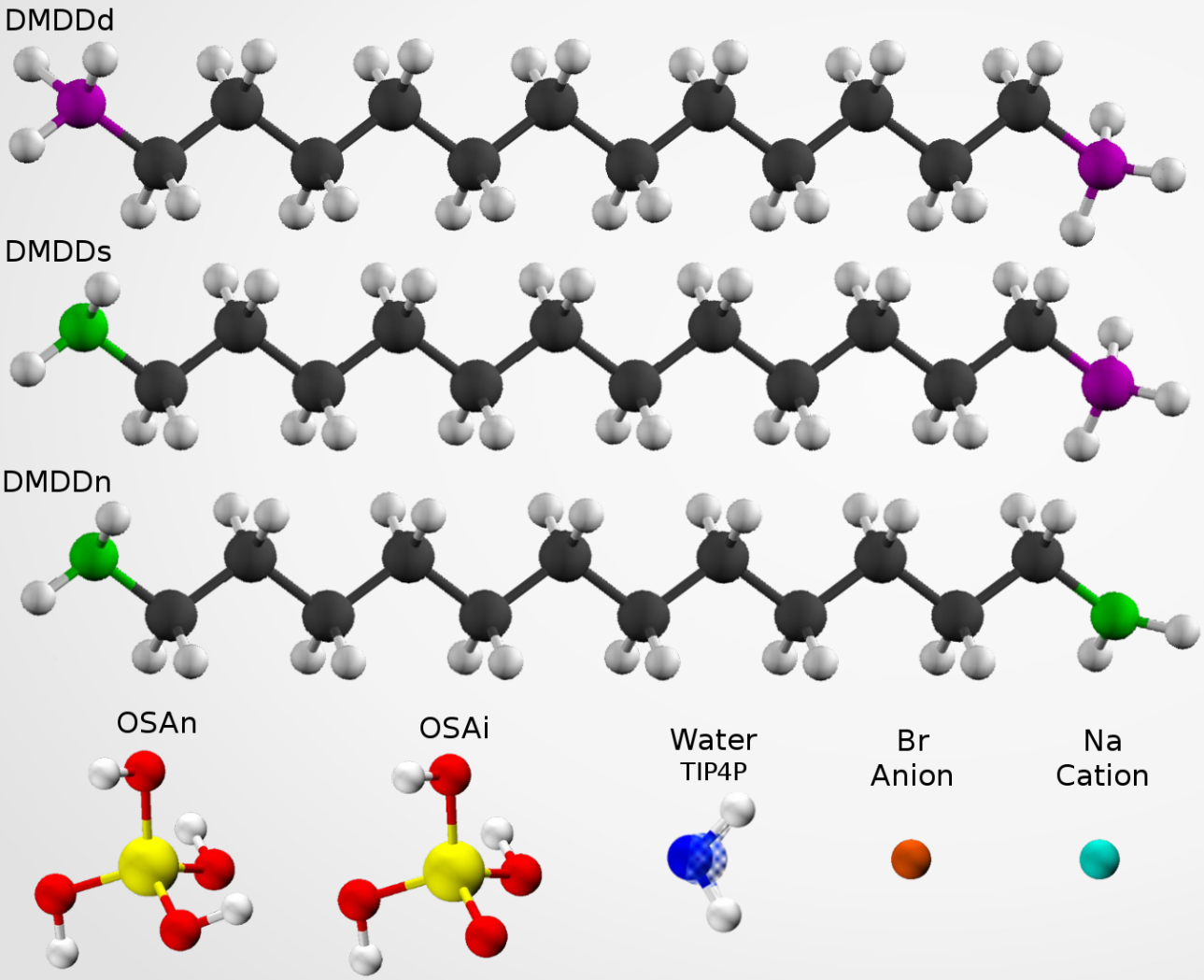
- Low no. Monte Carlo steps
- Great to initial potentials
- No cross-correlations

Inverse Monte Carlo

- More reliable potentials
- Cross-correlations
- High no. Monte Carlo steps



Atomistic Model



Analysis Objectives

- Box size
- Concentration
- pH

Atomistic Simulations

- NPT ensemble
- Over 100 ns

CG: Bead Size and Concentration

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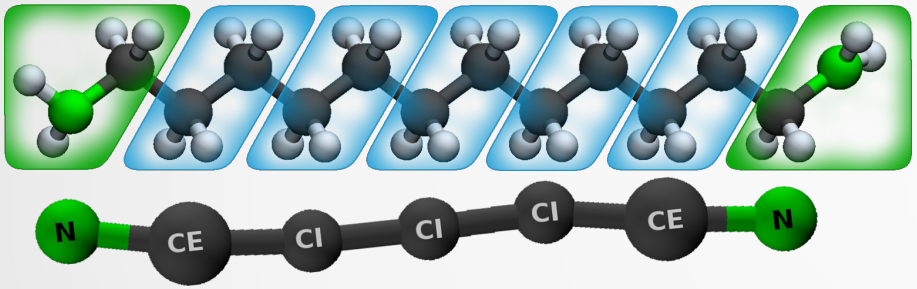
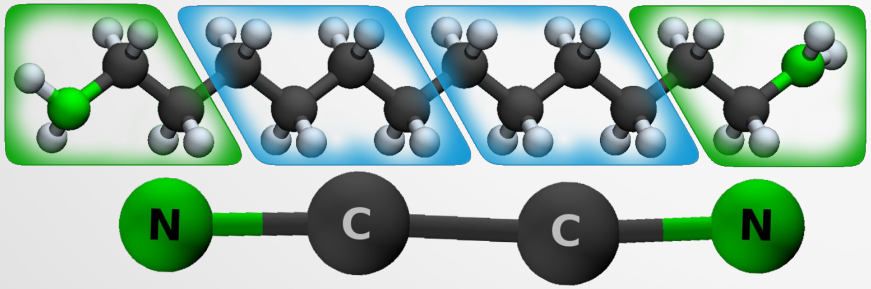
Multiple Models

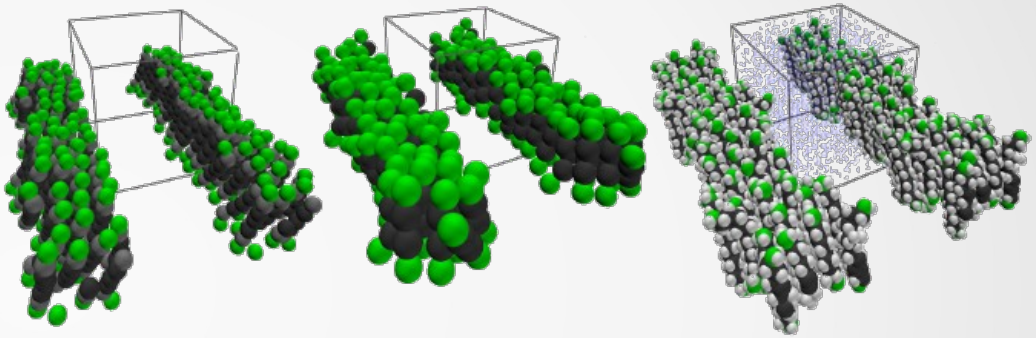
- Model 1:



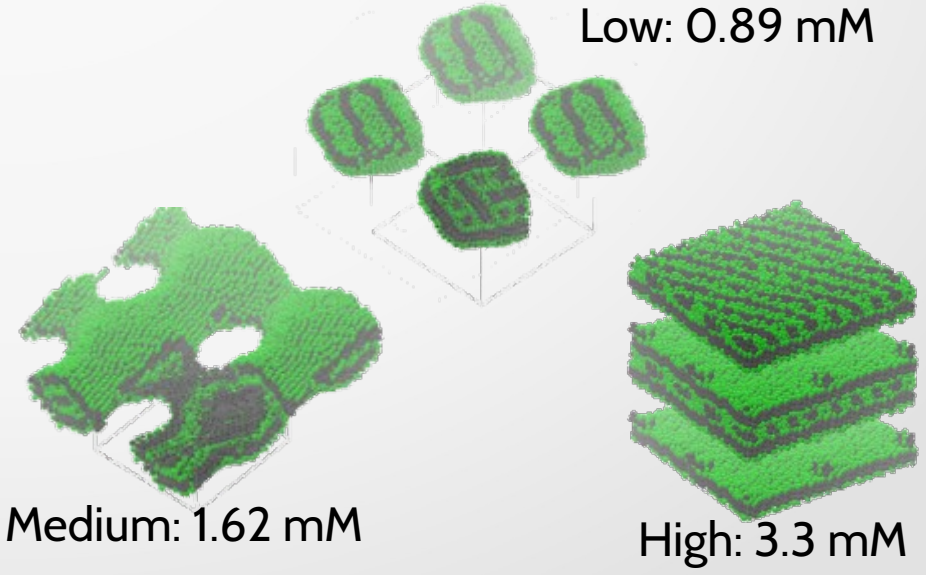
- Model 2:



Reproduction test:



Multiple Concentrations



CG: Charged Systems

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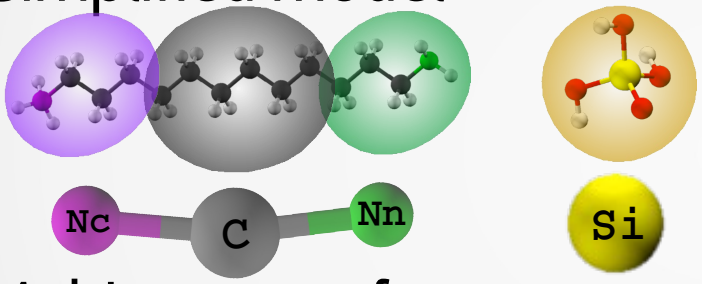
New Techniques for process efficiency

- Simplified model

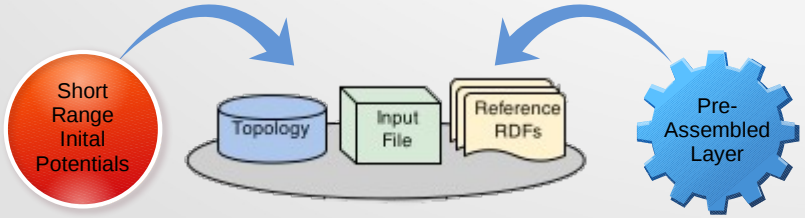


- Multi-states reference

  Short range reference: ~30 nm box

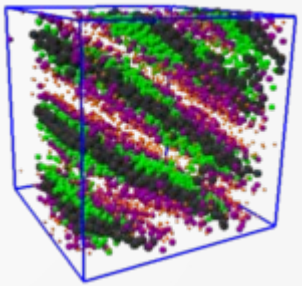
  Long range reference: > 42 nm box

- Changes on MagiC inputs

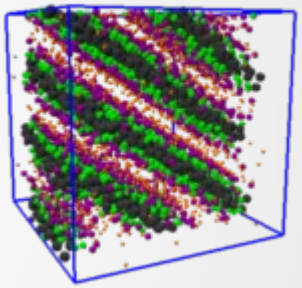


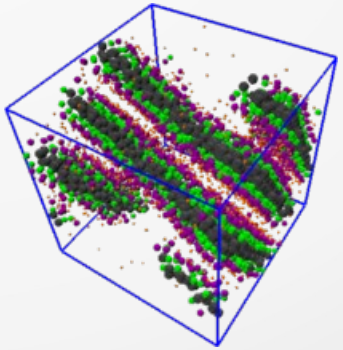
Influence of Electrostatic forces

Integrated

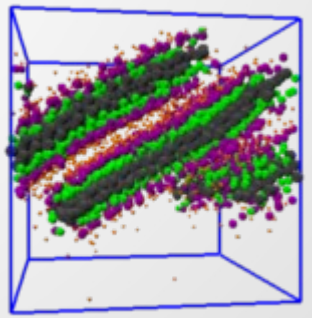


Short-range





Long-range



PME

CG: Silica surfactant system

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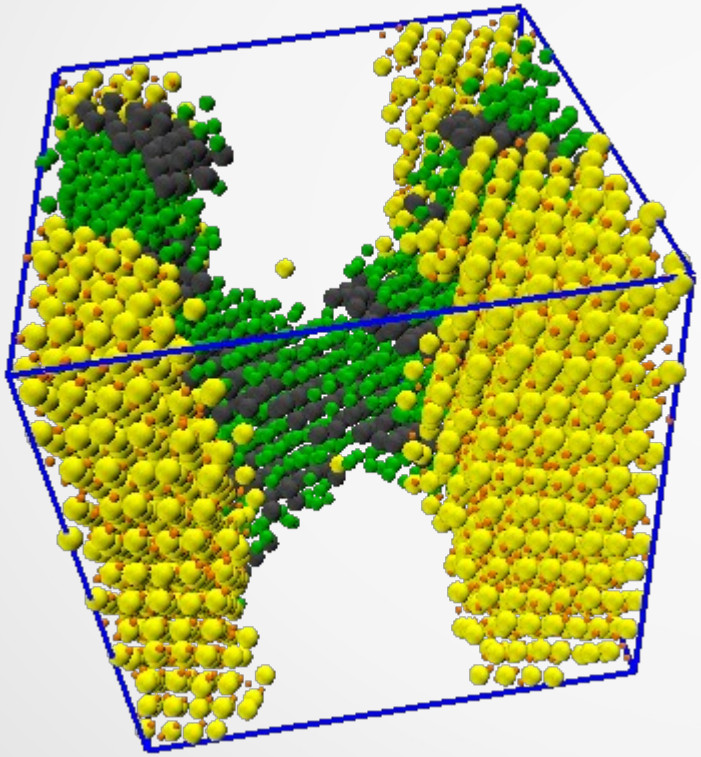
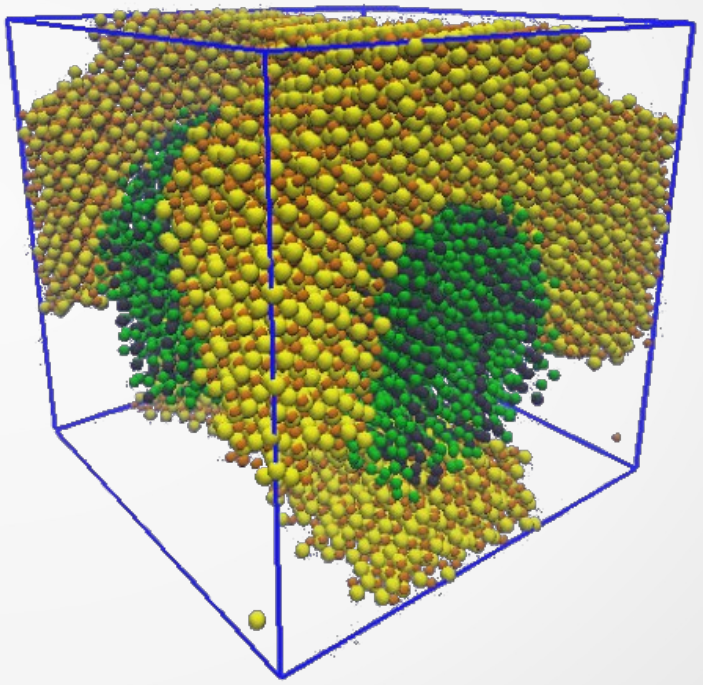
Ionic silica (OSAi) with neutral surfactant (DMDDn): Very High pH





Conclusion

- CG potentials are a feasible option
- Silica model still need improvements
- MagiC technique is very flexible
- Atomistic reference has deep influence in CG model

Ideas for the future

- Mixed CG model
- Multi-state potentials
- More focus in pH value

Any Questions?

Thank You!