DEPARTMENT OF CHEMICAL & PROCESS ENGINEERING

University of Strathclyde Engineering

Computer-aided Design of Bio-inspired Nanoporous Silica Materials

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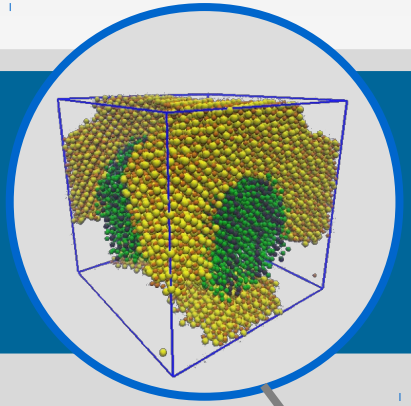
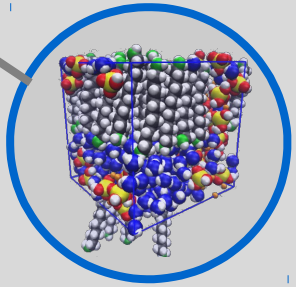


MagiC

GROMACS FAST. FLEXIBLE. FREE.



Silica-surfactant materials

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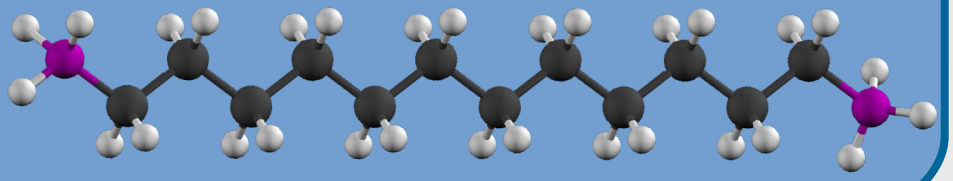
Highly Structured Materials

High Porosity
High Surface area

Generated by

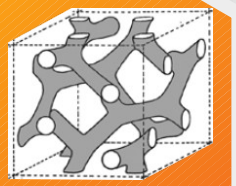
MSU-V

1,2-diaminododecane



Synthesis

MCM-50



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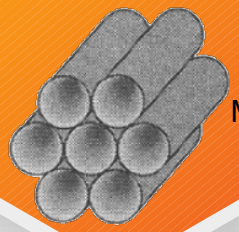
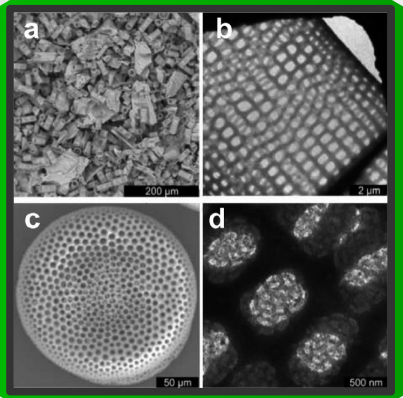


MCM-41

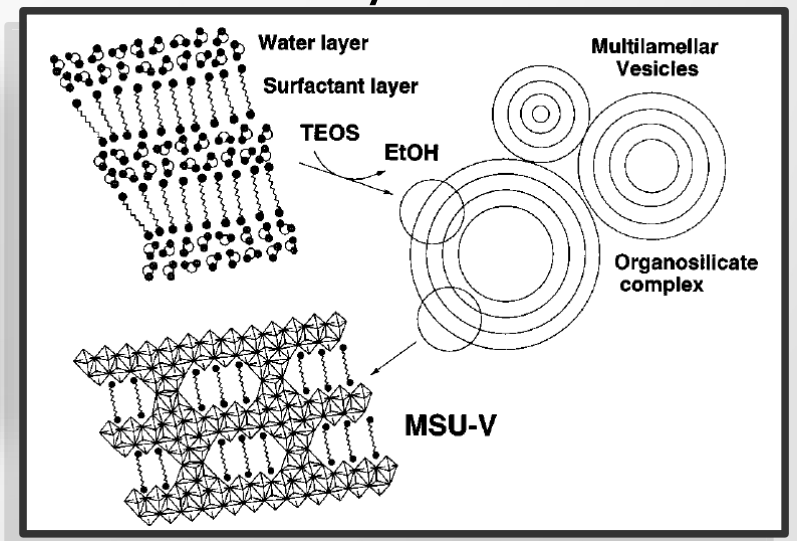
DOI:10.1039/C3CS60016E

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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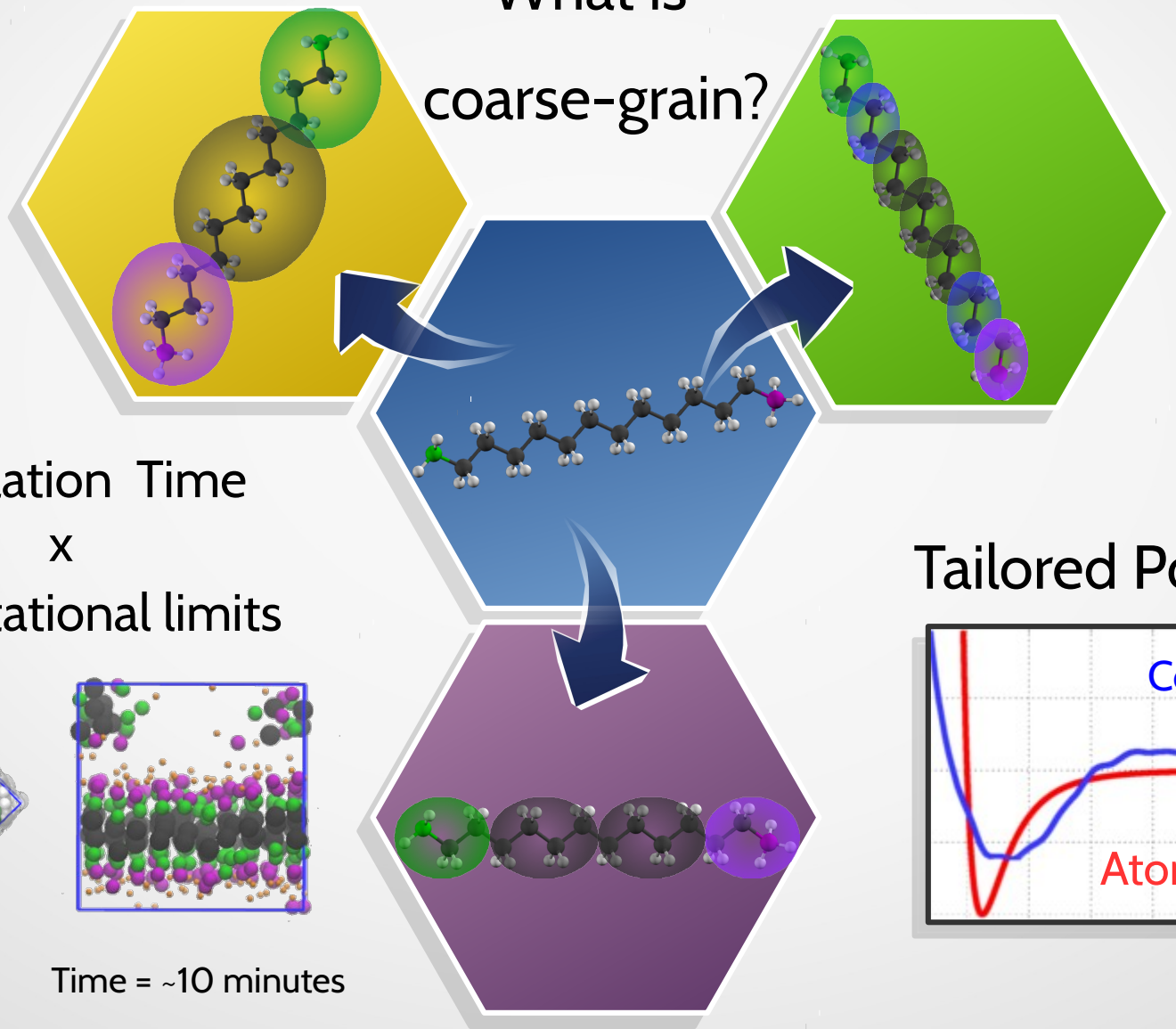
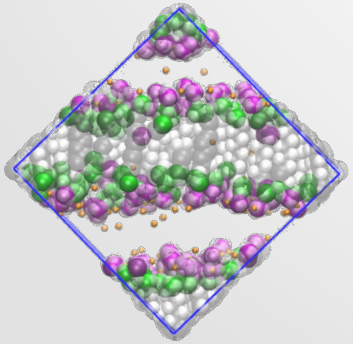
What is coarse-grain?



Simulation Time
x
Computational limits



Time = ~1,5 days

Time = ~10 minutes

Tailored Potentials

MagiC: a systematic method

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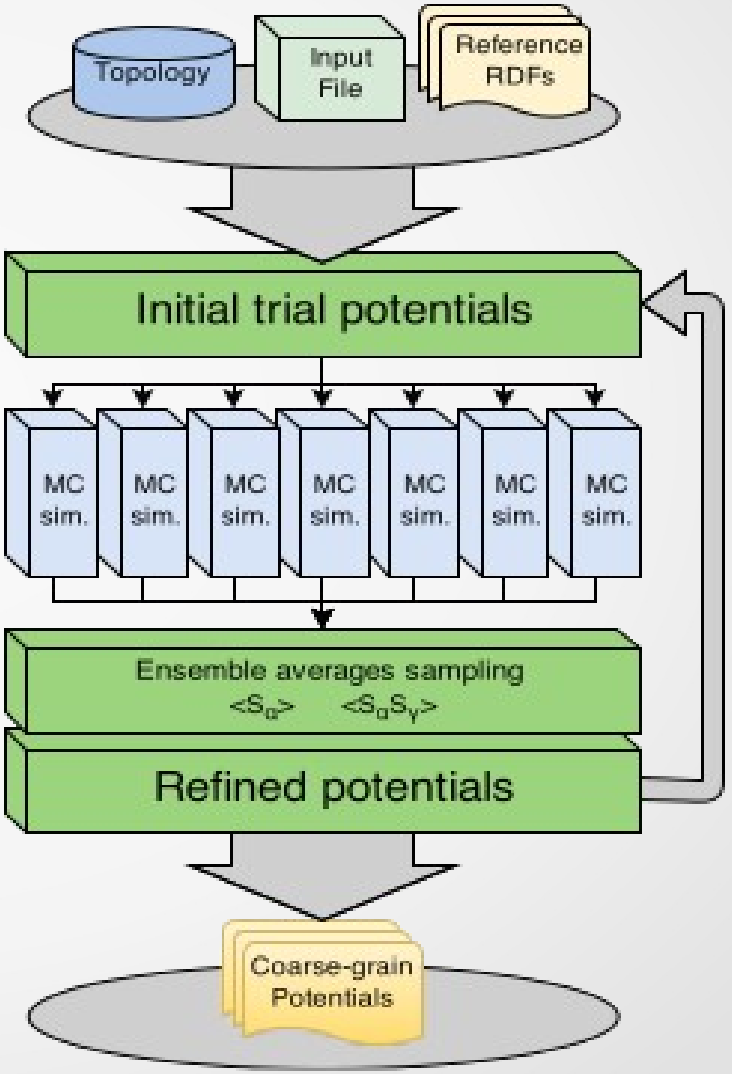
Boltzmann inversion

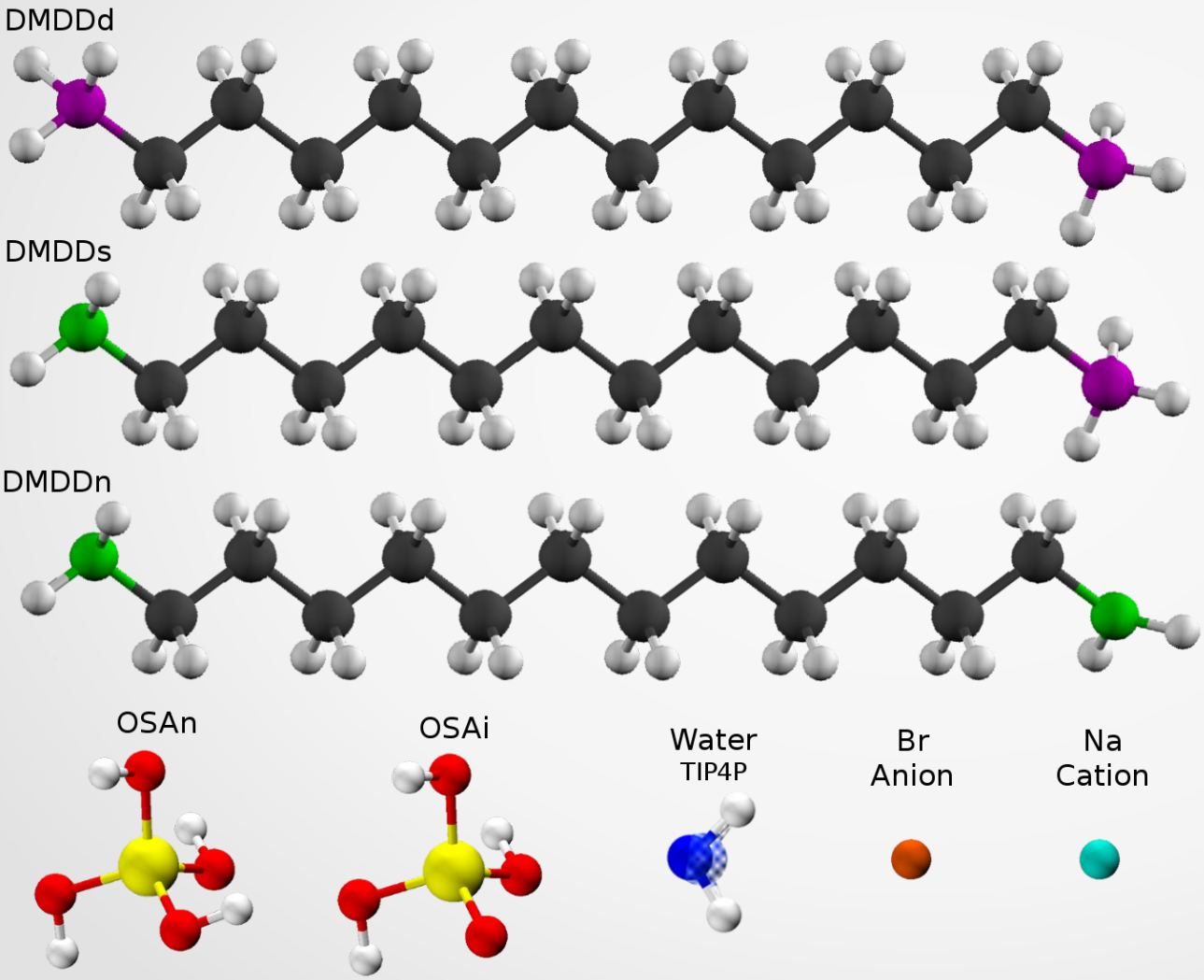
- Low no. Monte Carlo steps
- Great to initial potentials
- No cross-correlations

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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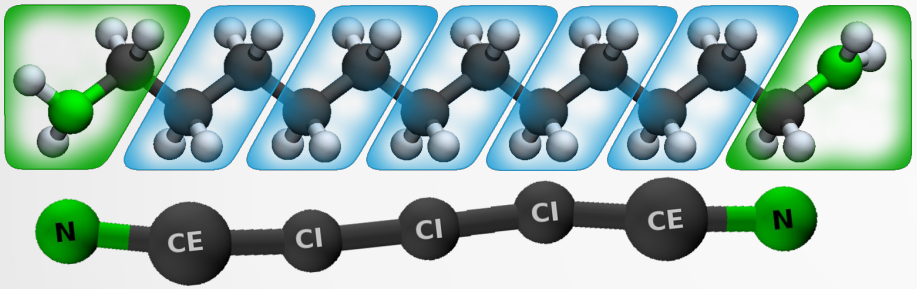
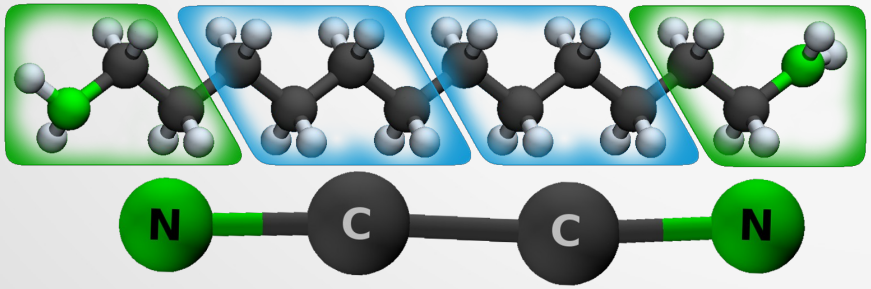
Multiple Models

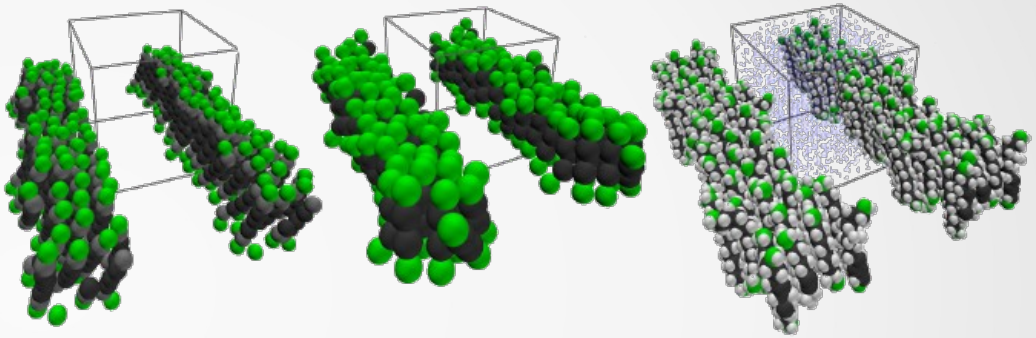
- Model 1:



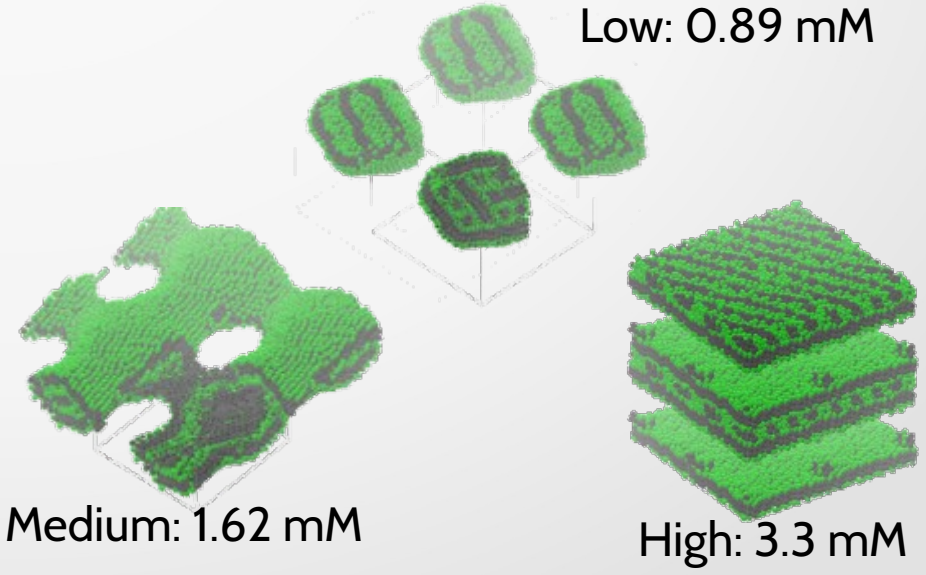
- Model 2:



Reproduction test:



Multiple Concentrations



CG: Charged Systems

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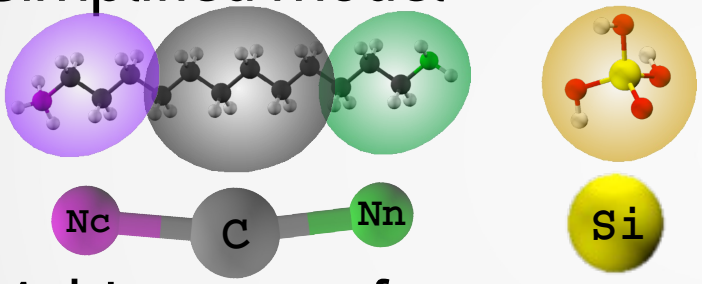
New Techniques for process efficiency

- Simplified model

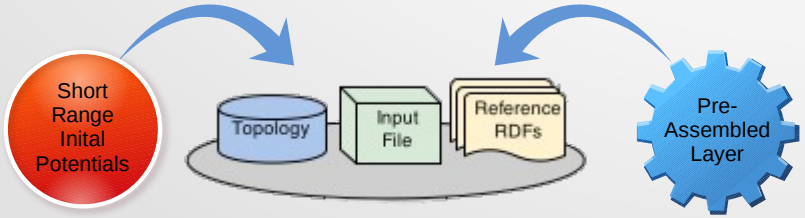


- Multi-states reference

  Short range reference: ~30 nm box

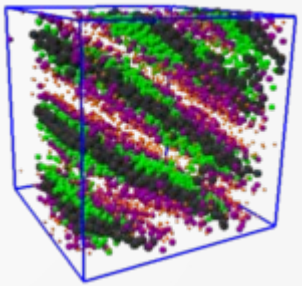
  Long range reference: > 42 nm box

- Changes on MagiC inputs

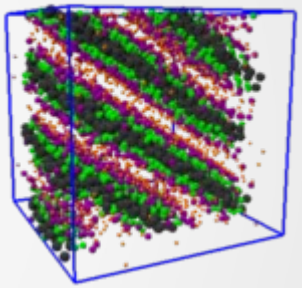


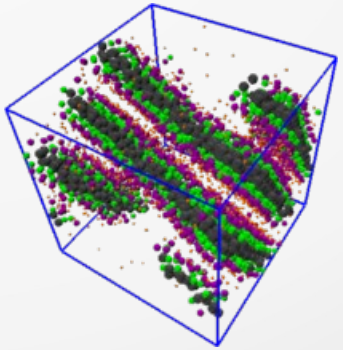
Influence of Electrostatic forces

Integrated

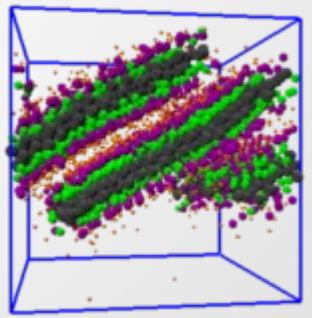


Short-range





Long-range



PME

CG: Silica surfactant system

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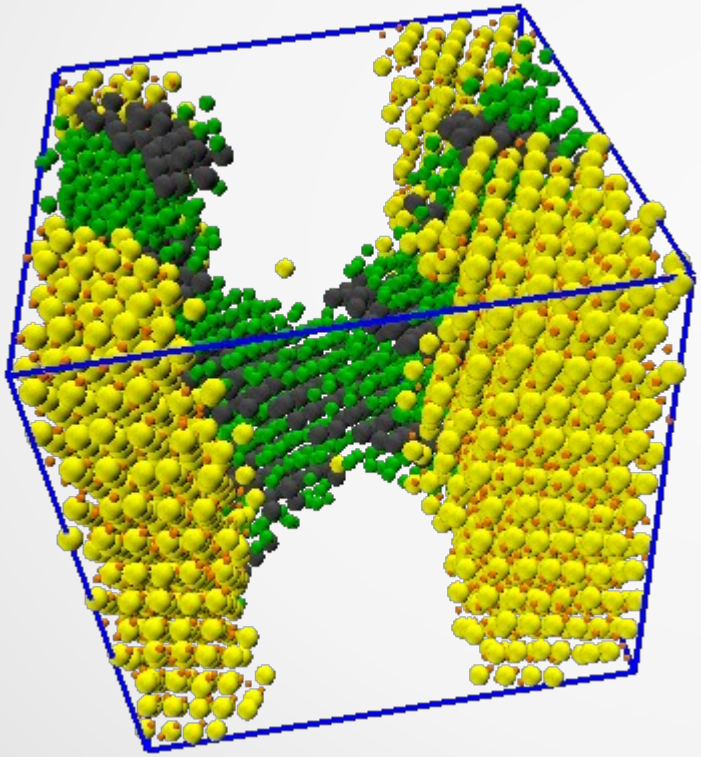
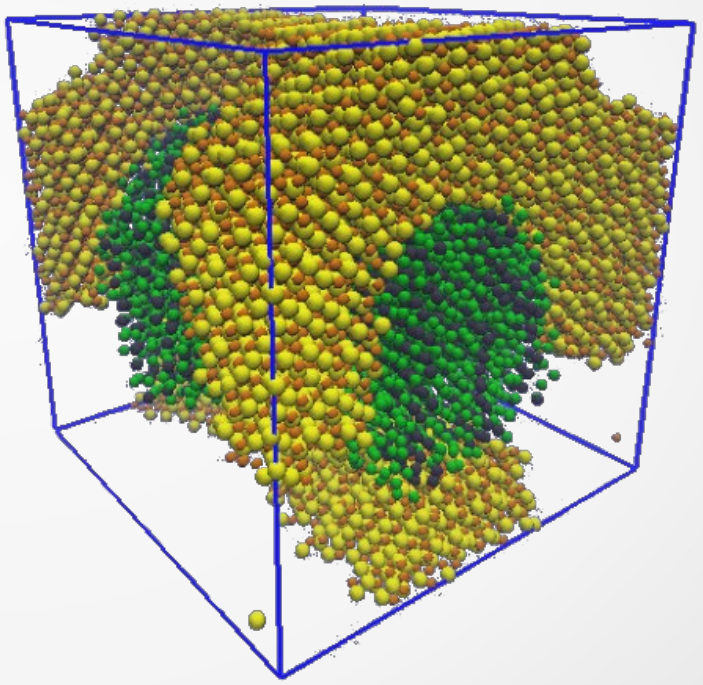
Ionic silica (OSAi) with neutral surfactant (DMDDn): Very High pH





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