DEPARTMENT OF CHEMICAL & PROCESS ENGINEERING

University of Strathclyde Engineering

# Computer-aided Design of Bio-inspired Nanoporous Silica Materials


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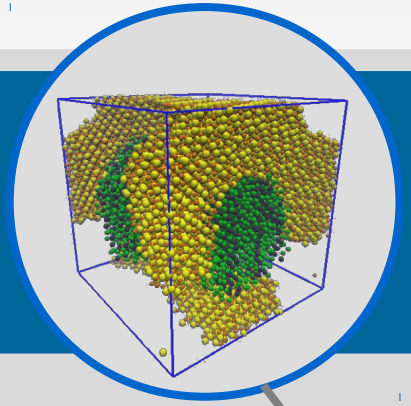
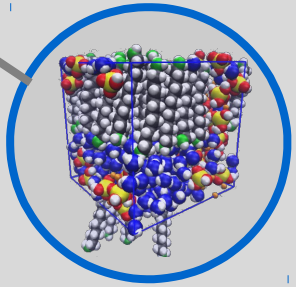


MagiC

GROMACS FAST. FLEXIBLE. FREE.



# Silica-surfactant materials

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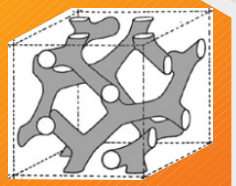
Highly Structured Materials

High Porosity
High Surface area

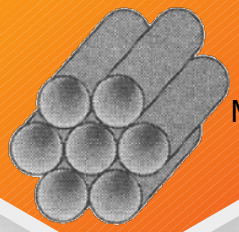
Generated by

## Synthesis

MCM-50

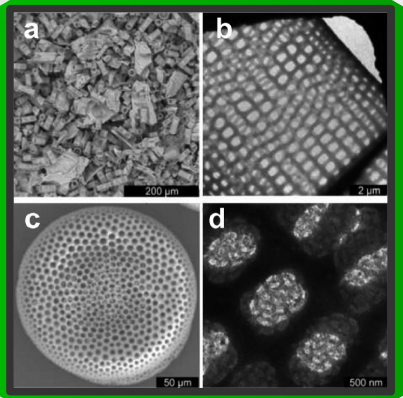


MCM-48



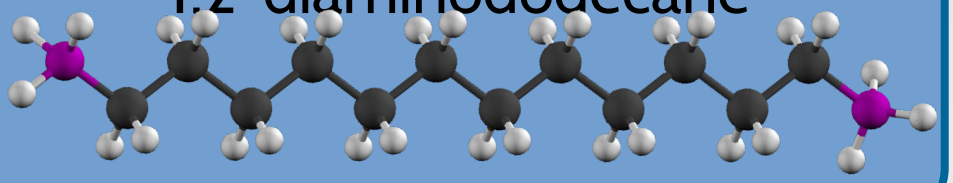
MCM-41

## Nature

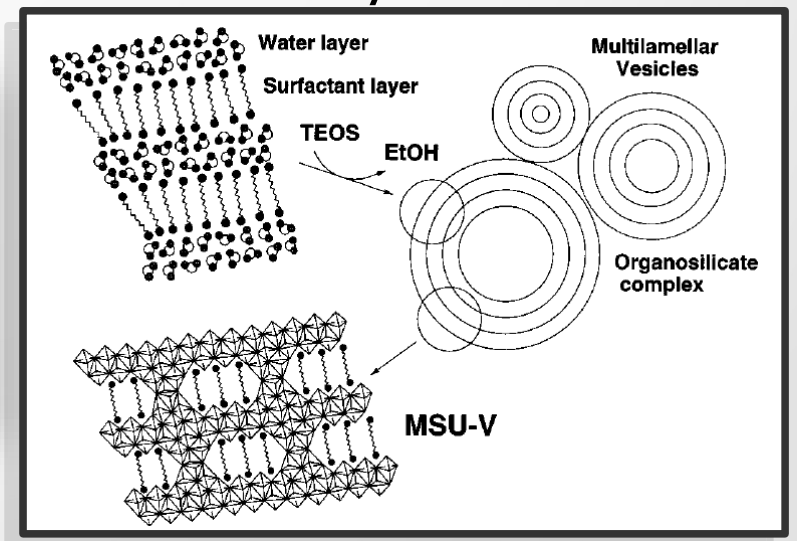



## MSU-V

1,2-diaminododecane



## Self-Assembly structure



# 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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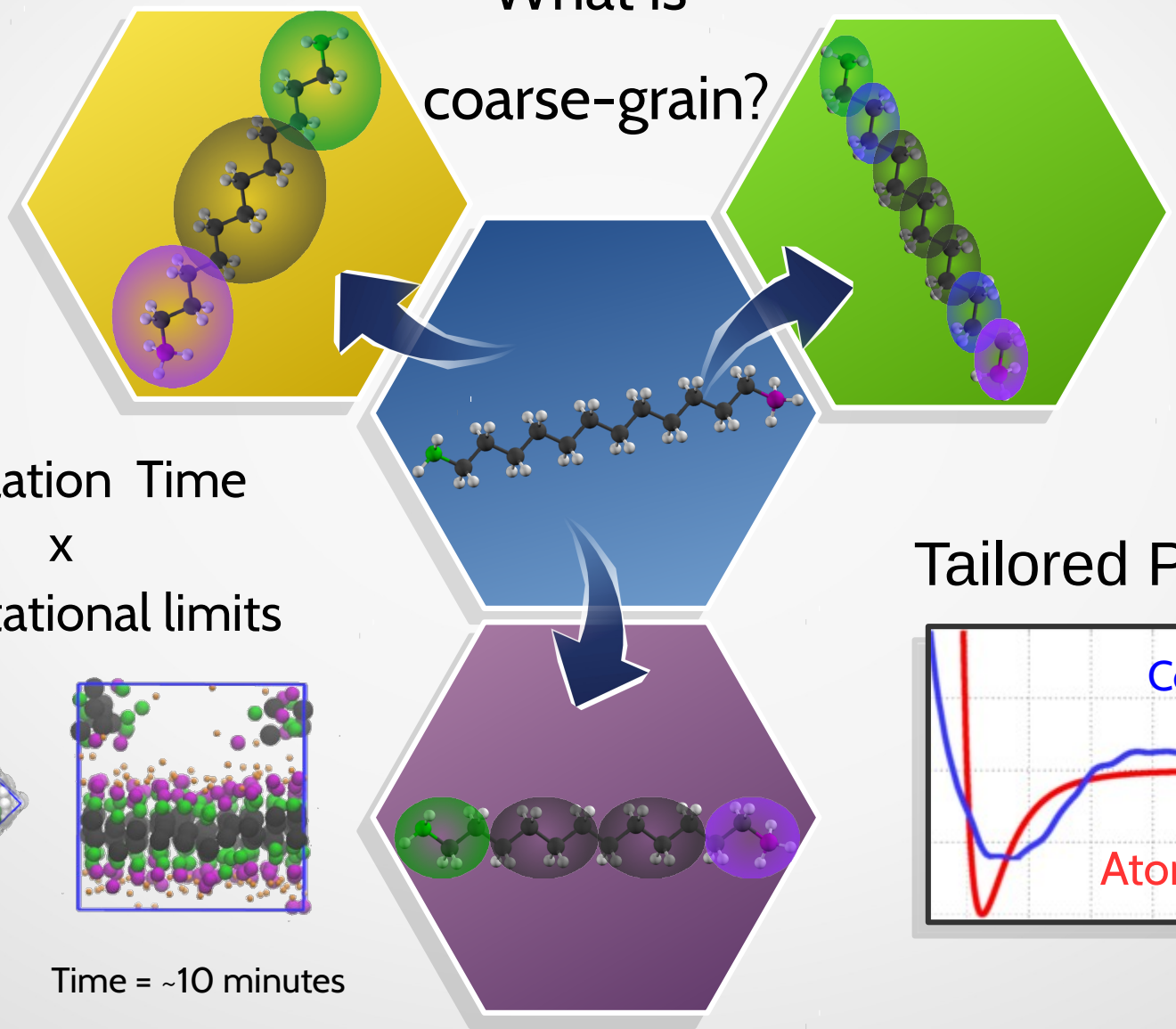
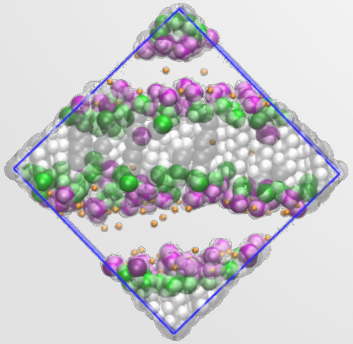
What is coarse-grain?



Simulation Time
x
Computational limits



Time = ~1,5 days

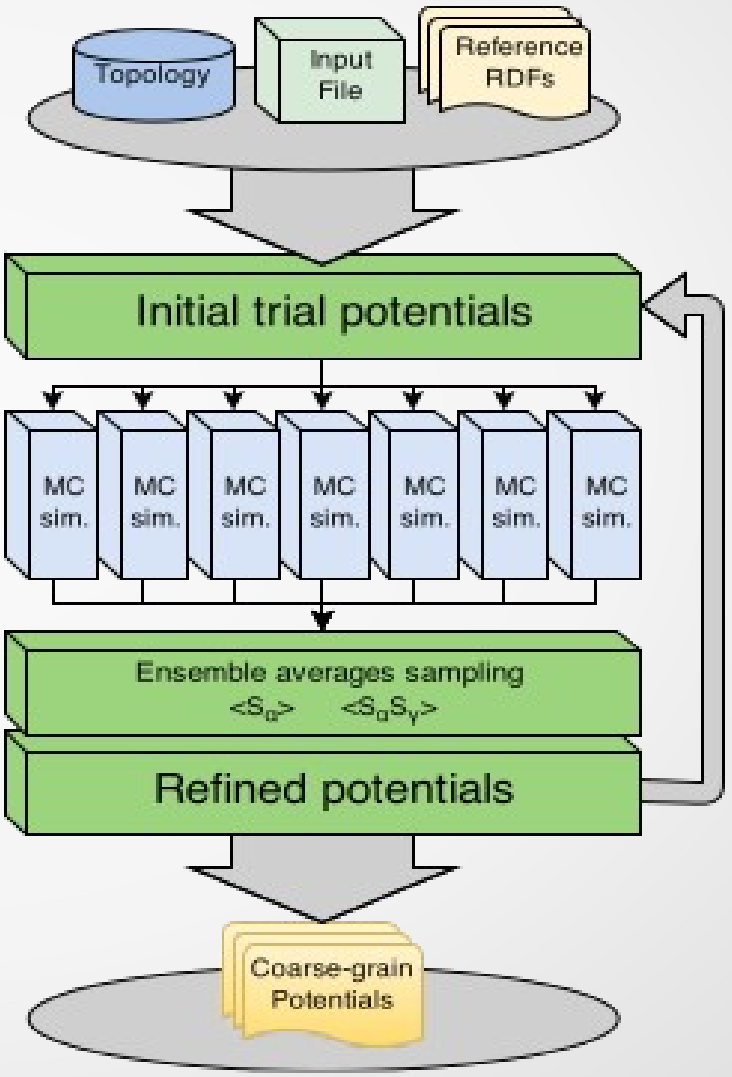


Time = ~10 minutes

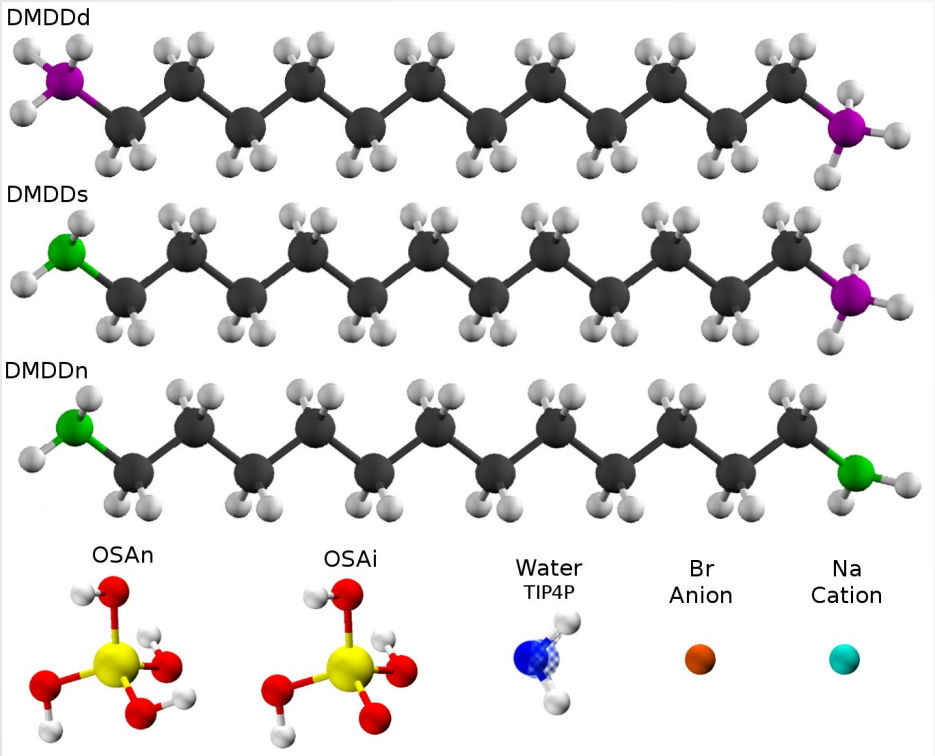
Tailored Potentials

# MagiC: a systematic method

- Boltzmann inversion
- Inverse Monte Carlo



# Atomistic Model




- Concentration
- pH
- Equilibrium Structure

- Standardized simulations
  - NPT
  - Over 100 ns

# CG Modelling: Bead Size and Concentration

- Multiple Models
  - Model 1:


  - Model 2:


- Multiple Concentrations
  - Low
  - Medium
  - High

# CG Modelling: Charged Systems

- New Techniques for process efficiency
  - Simplified model

  - Multi-states reference
  - Changes on MagiC inputs

- Influence of Electrostatic forces
  - Integrated Electrostatics
  - Short range Electrostatics
  - Long range Electrostatics

# CG Modelling: Silica introduction

- Ionic silica with neutral surfactant
- Ionic silica with singly charged surfactant

# Conclusion

- (general conclusion)
- (still need to think)

- Ideas for the future
  - Artificial CG model
  - Multi-state IBI
  - More focus in pH value