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Classical Forcefield-based Methods

Marianna Yiannourakou, Jörg-Rüdiger Hill
Materials Design

Oct 12, 2021

Materials Design UGM

UGM 2021

The Materials Design annual user event will be online again for 2021.

Plenary Speakers include:

Prof. Michele Parrinello
Prof. Georg Kresse
Prof. Richard Catlow

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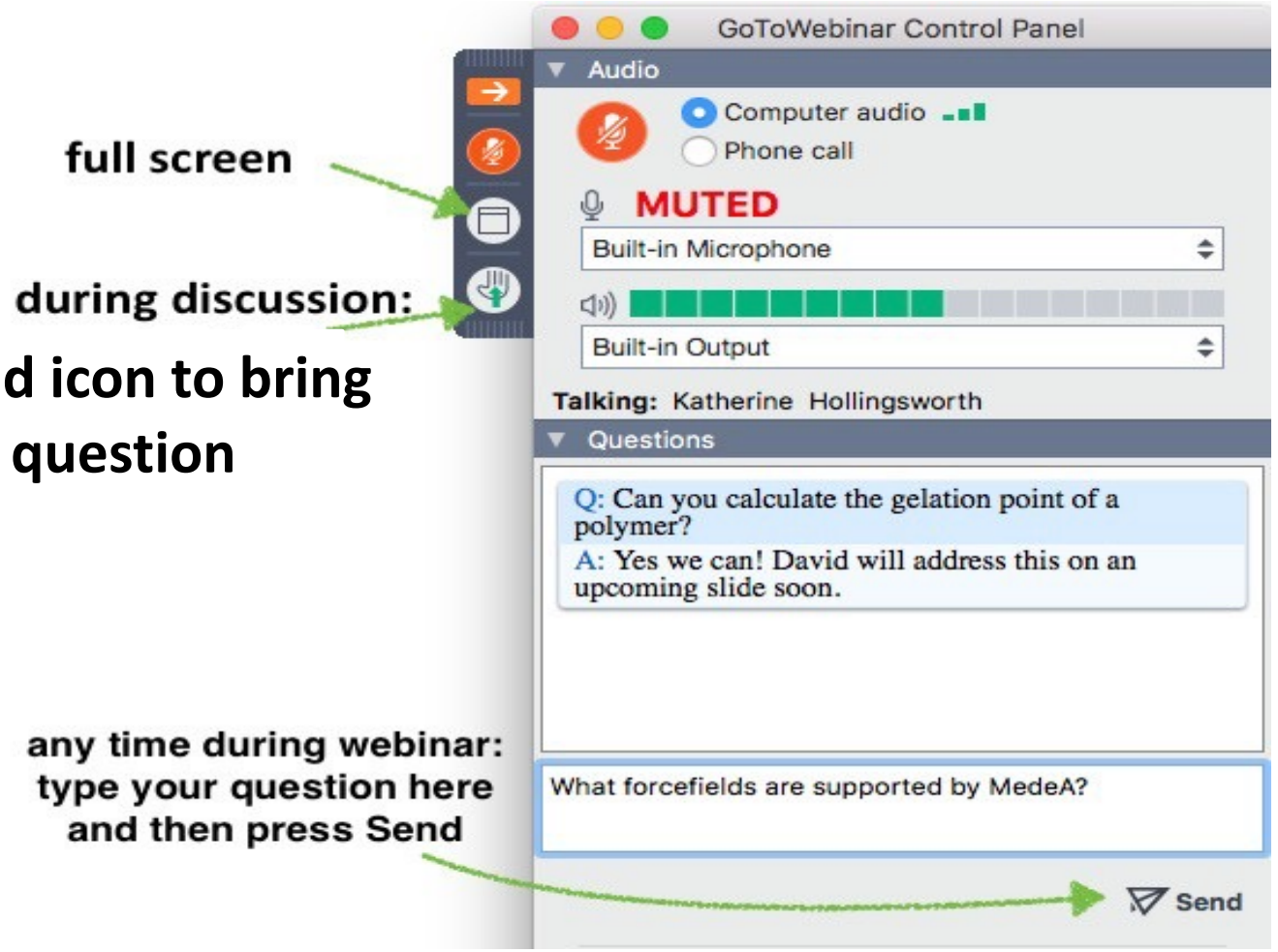
Materials Design UGM Training Sessions

- Tuesdays in this UGM series will feature online training sessions with members of the Materials Design Team
- Share the training sessions with your colleagues!
  - Registration details
    - https://ugm.materialsdesign.com
- We will be recording this session
  - Upcoming sessions are posted on the UGM site
  - Watch any of our earlier webinars anytime www.materialsdesign.com/webinars
- Audio issues
  - Log out and log back in again
  - Check your audio output
  - Google Chrome (most recent 2 versions) Mozilla Firefox (most recent 2 versions) Apple Safari (most recent 2 versions) Microsoft Edge (most recent 2 versions)

Please Ask Questions!



Use the raise hand icon to bring attention to your question

Training Session Instructors

Dr. Marianna Yiannourakou ***Dr. Jörg-Rüdiger Hill*** ***Dr. Ray Shan***

Materials Design Support Team

René Windiks ***Thomas Nilson*** ***Shubham Pandey*** ***David Reith*** ***Ray Shan***

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Classical Forcefield-based Methods:

MedeA GIBBS and Monte Carlo Methods

Marianna Yiannourakou

Materials Design

Oct 12, 2021

Outline

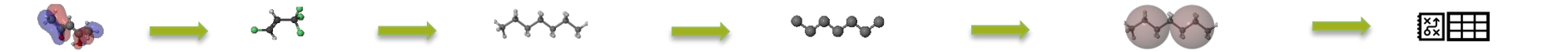
- Short overview of Forcefield simulations
- Forcefields in *MedeA*
- Solubility of gases in solids - Grand Canonical Monte Carlo (GCMC) simulations with *MedeA GIBBS*
- Solubility of gases in liquids – NPT Monte Carlo simulations & widom test insertions with *MedeA GIBBS*

GIBBS: IFP Energies Nouvelles, Rueil-Malmaison & Laboratoire de Chimie-Physique, Université Paris Sud, CNRS, France.

Ungerer, P. ; Tavitian, B. ; Boutin, A. *Applications of Molecular Simulation in the Oil and Gas Industry : Monte Carlo Methods*, Editions Technip - IFP Publications, Paris, France, 2005.

Short overview of Forcefield simulations

Levels of description / Access to information



QM

- All or valence electrons

Semi-empirical QM

- valence electrons
- electron-electron interactions empirically parameterized

Forcefield (atomistic)

- All atoms
- Non-reactive & reactive forcefields

Forcefield (united atoms)

- groups containing 1 heavy atom (CHx groups)
- non-reactive forcefields

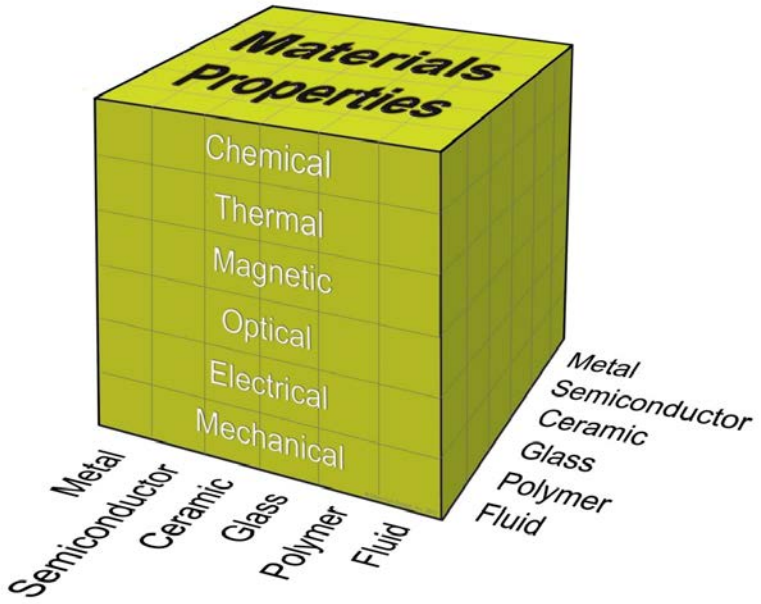
Forcefield (coarse-grained)

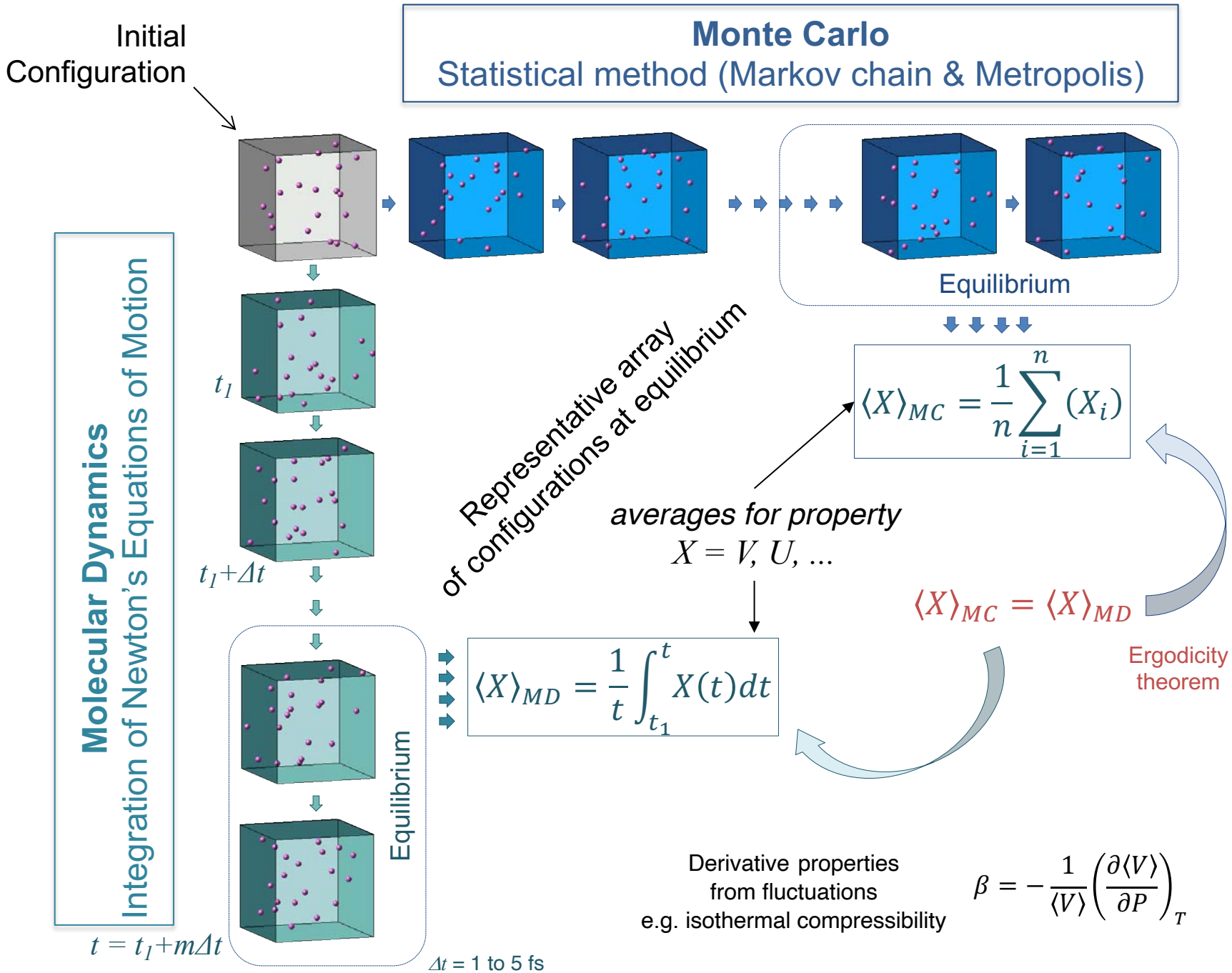
- beads containing 2-4 heavy atoms
- non-reactive forcefields

QSAR

- Correlations

Prediction of materials properties of engineering value



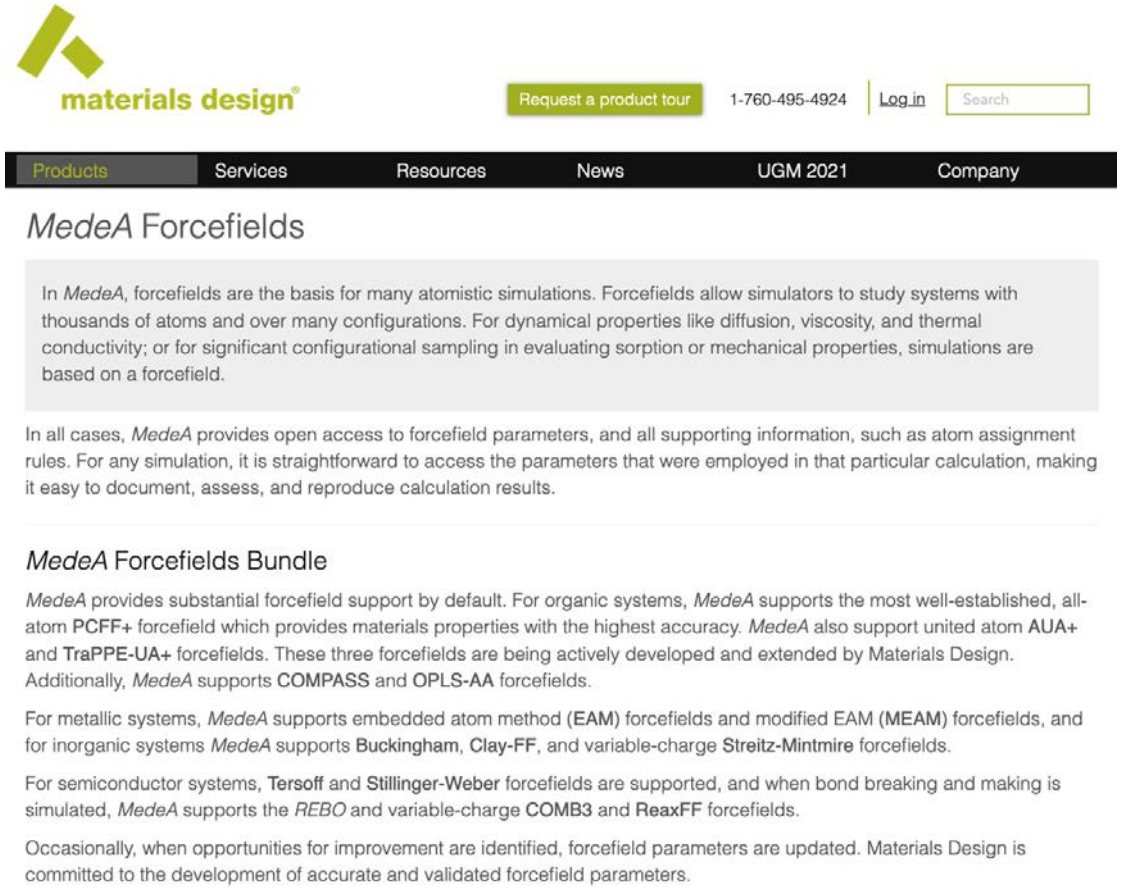

Initial Configuration
Monte Carlo
Statistical method (Markov chain & Metropolis)
Equilibrium
Representative array of configurations at equilibrium
$\langle X \rangle_{MC} = \frac{1}{n}\sum_{i=1}^{n}(X_i)$
averages for property
$X = V, U, \ldots$
$\langle X \rangle_{MC} = \langle X \rangle_{MD}$
Ergodicity theorem
$\langle X \rangle_{MD} = \frac{1}{t}\int_{t_1}^{t} X(t)dt$
Molecular Dynamics
Integration of Newton's Equations of Motion
t_1
$t_1+\Delta t$
$t = t_1+m\Delta t$
Equilibrium
Δt = 1 to 5 fs
$m\Delta t$ = 1 to 20 ns
Derivative properties from fluctuations
e.g. isothermal compressibility
$\beta = -\frac{1}{\langle V \rangle}\left(\frac{\partial \langle V \rangle}{\partial P}\right)_T$

Forcefields in MedeA

Forcefields in *MedeA*

- All-atom, e.g. PCFF+, OPLSAA, Compass, ClayFF, CVFF aug, GAFF…
- United atom, e.g. AUA/AUA+, TraPPE-UA+
- Coarse-Grained, e.g. SPICA, MARTINI, MARTINI 3.0
- ReaxFF
- Comb3
- EAM
- MLPs

- Use of existing forcefields (from literature)
- Introduce forcefields (from literature)
- Create forcefields (*MedeA MLPG* & *MedeA FFO*)



https://www.materialsdesign.com/forcefields

Solubility of gases in solids - Grand Canonical Monte Carlo (GCMC) simulations with MedeA GIBBS

Microporous adsorbent of rigid structure

Insertion-deletion Monte Carlo moves include the interactions with the solid as an additional contribution to the potential energy U

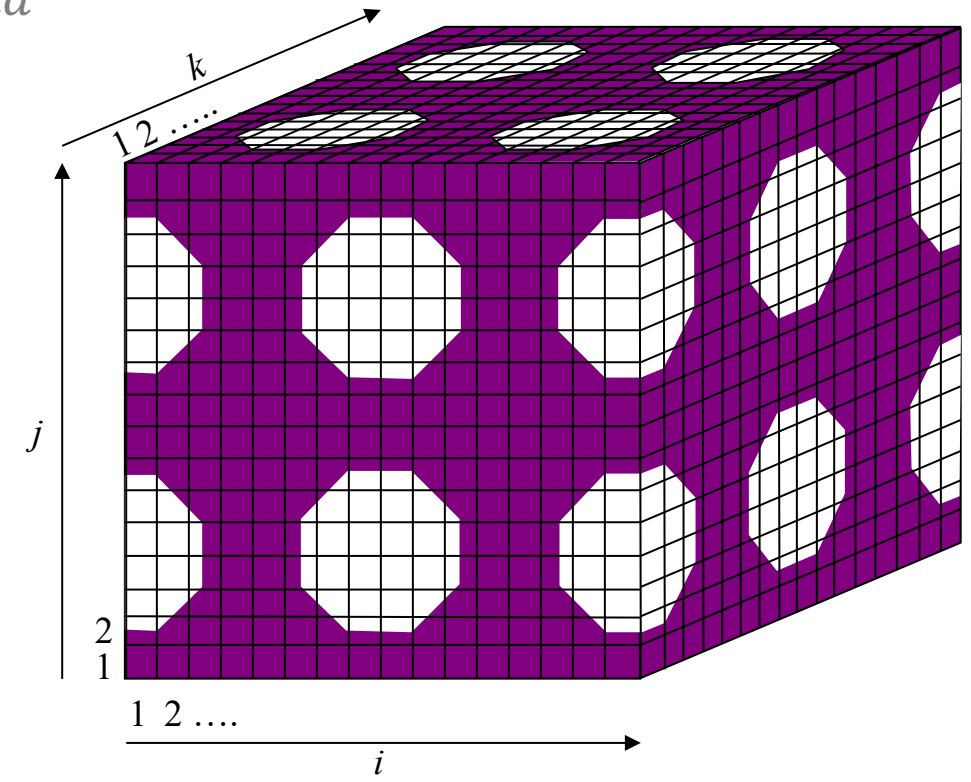
$$U = U_{mol-mol} + U_{mol-solid} + U_{solid-solid}$$

Internal energy of molecules and intermolecular energy

Interaction energy between the molecules and the adsorbent

Neglected (no solid deformation)

Computation of the potential energy field on a grid U(i,j,k) allows to save computing time

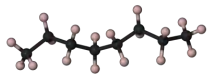


Characterization and Sorption

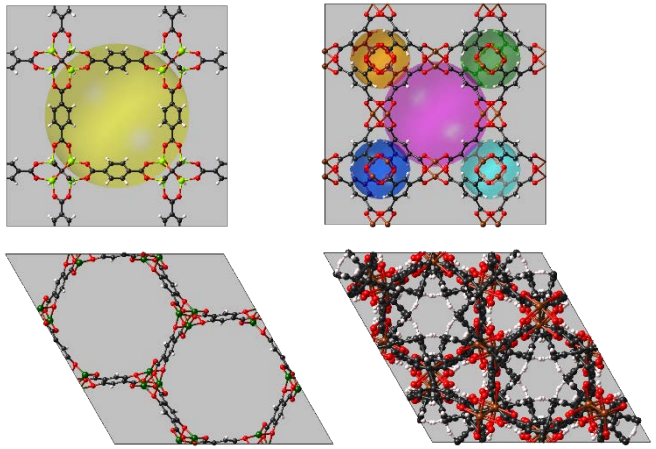
1 Create a system

- Build
  - Molecular Builder
  - Crystal Builder
  - Nano-particle/tube/wrap Builder
  - Surface Builder
  - Polymer Builder
  - Thermoset Builder
- Get from InfoMaticA
  - ICSD, COD, Pearsons, NIST, user
- Import from external file
  - read-in (sci, cif, xyz, car etc)

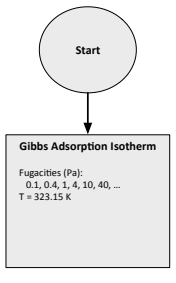
Adsorbate

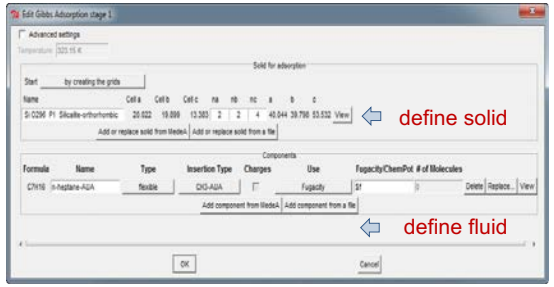


Adsorbent



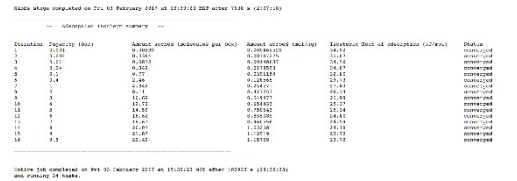
2 Run MC simulations to get sorption isotherms



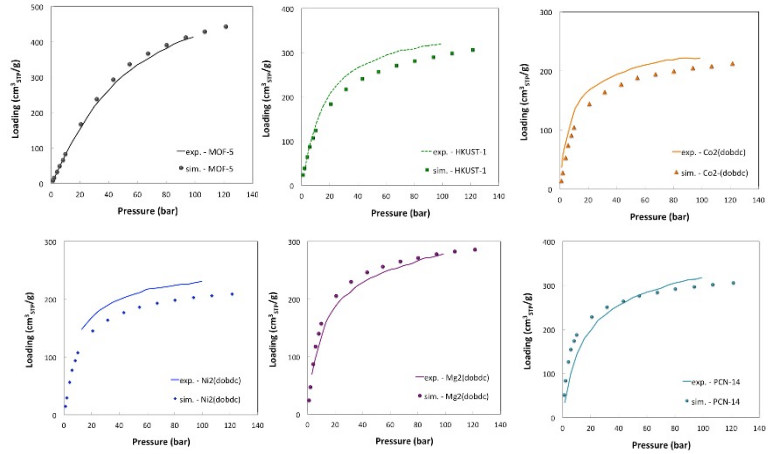


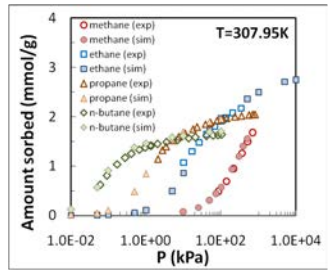
- Submit a single job to get an entire isotherm
- Run adsorption & desorption paths
- Chose to have mobile or immobile cations in a zeolite

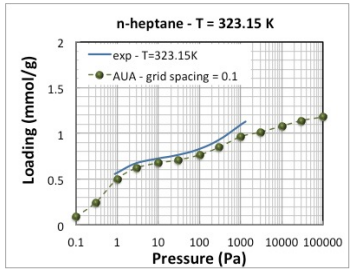
3 Get Results



- Adsorption/desorption isotherms
- Heats of adsorption
- Surface Area (BET, Langmuir)
- Pore Volume (pyknometry)







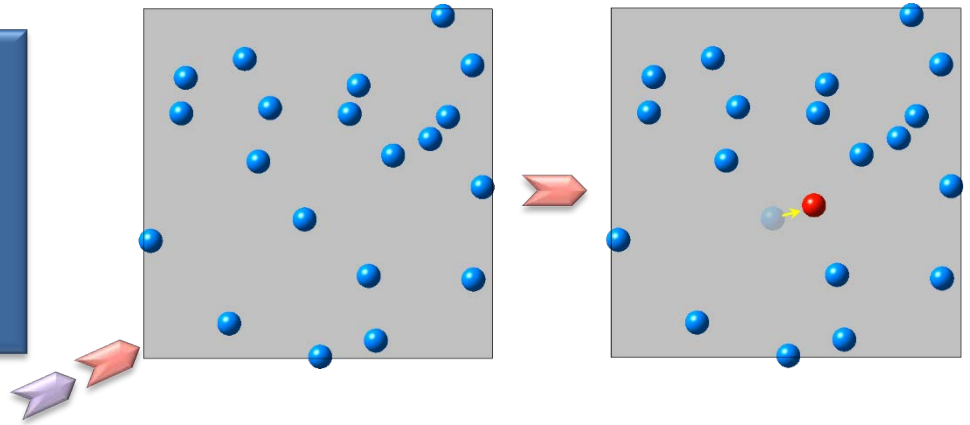
Solubility of gases in liquids – NPT Monte Carlo simulations & widom test insertions with MedeA GIBBS

Widom test insertions in the NVT & NPT ensembles

CANONICAL ENSEMBLE:
(NVT)

Input / Imposed Quantities:

N (number of molecules) → constant
V (Volume) → constant
T (Temperature) → constant

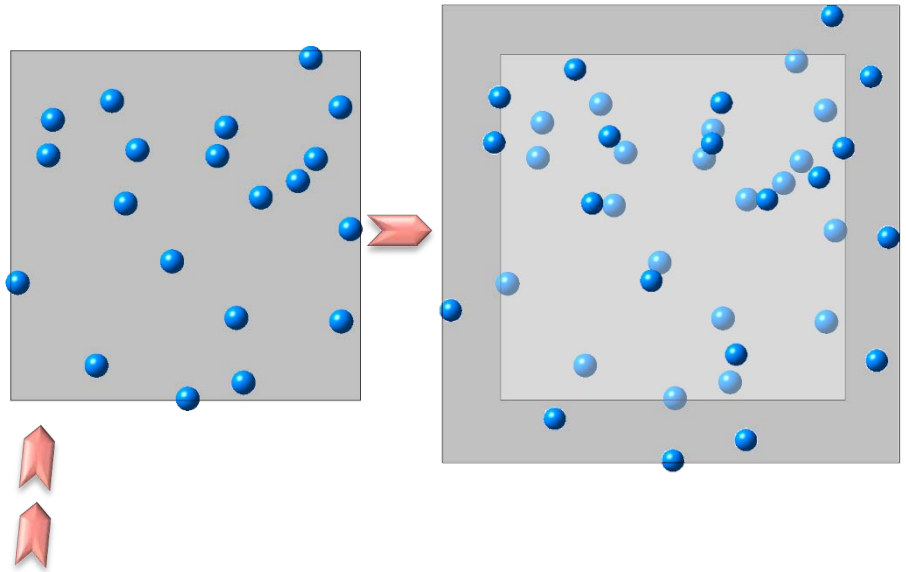


- Translation (atoms & molecules)
- Rotation (molecules)
- Internal moves (flexible molecules)

ISOTHERMAL-ISOBARIC ENSEMBLE:
(NPT)

Input / Imposed Quantities:

N (number of molecules) → constant
P (Pressure) → constant
T (Temperature) → constant

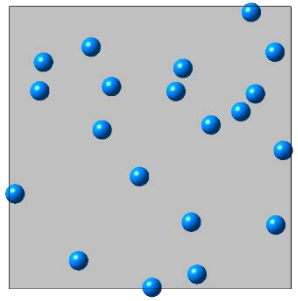


- Translation (atoms & molecules)
- Rotation (molecules)
- Internal moves (flexible molecules)
- Volume change (expansion/ compression)

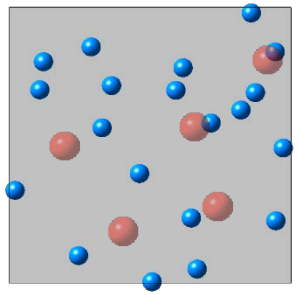
Widom test insertion:

- in random positions,
- energy recorded
- insertion move never accepted

B. Widom, "*Some Topics in the Theory of Fluids*", J. Chem. Phys. **39**, p. 2808 (1963)



Test insertions



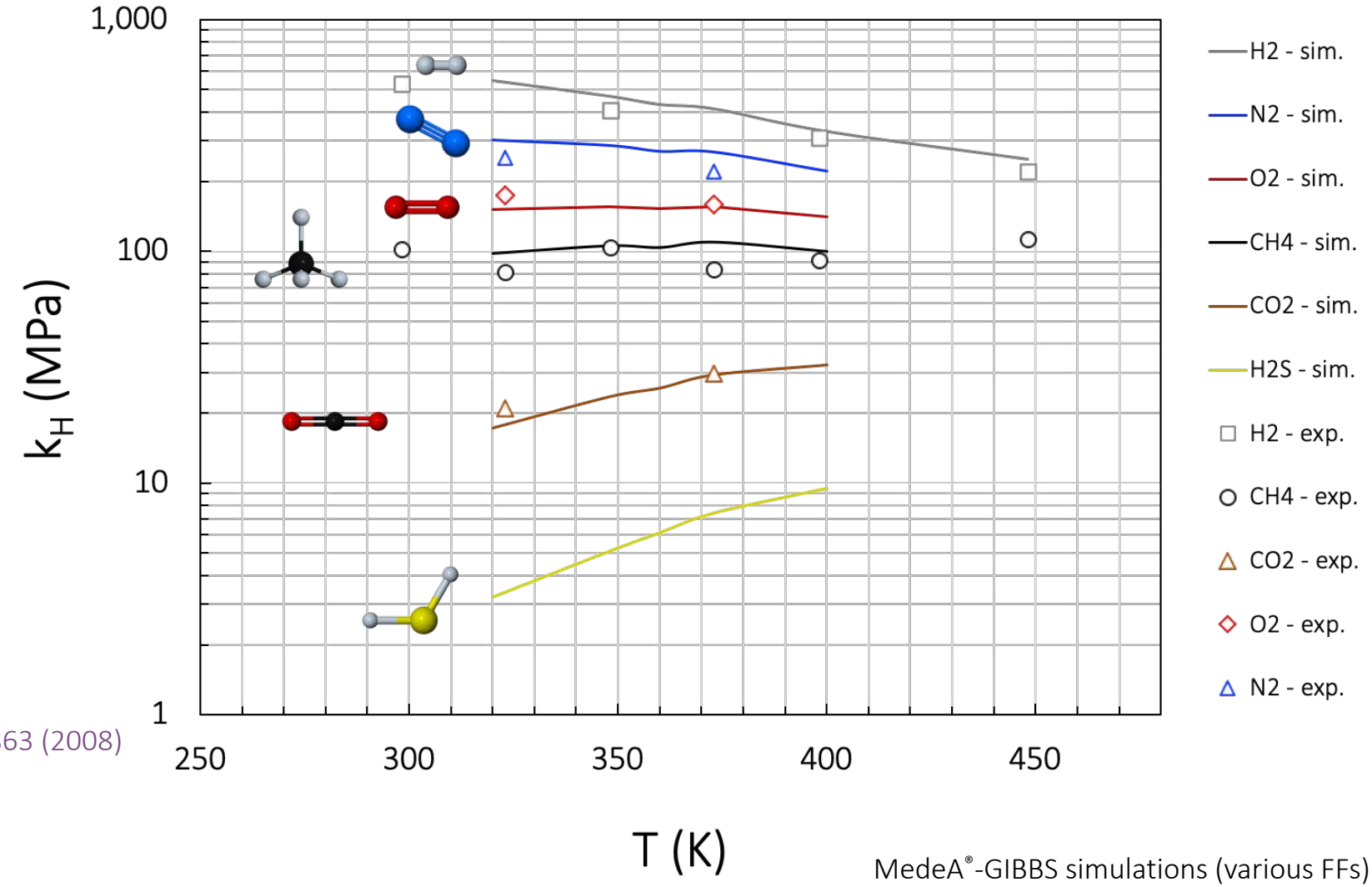
Henry Solubility Constants in Ethanol

Henry's law: $P_i = K_{H,i} \cdot x_i$

where:

- i is the solute,
- P_i is the partial pressure of i
- $K_{H,i}$ is the Henry constant of i
- x_i is the molar fraction of i in the mixture

$K_{H,i}$ → obtained from sim. (Widom test insertions)



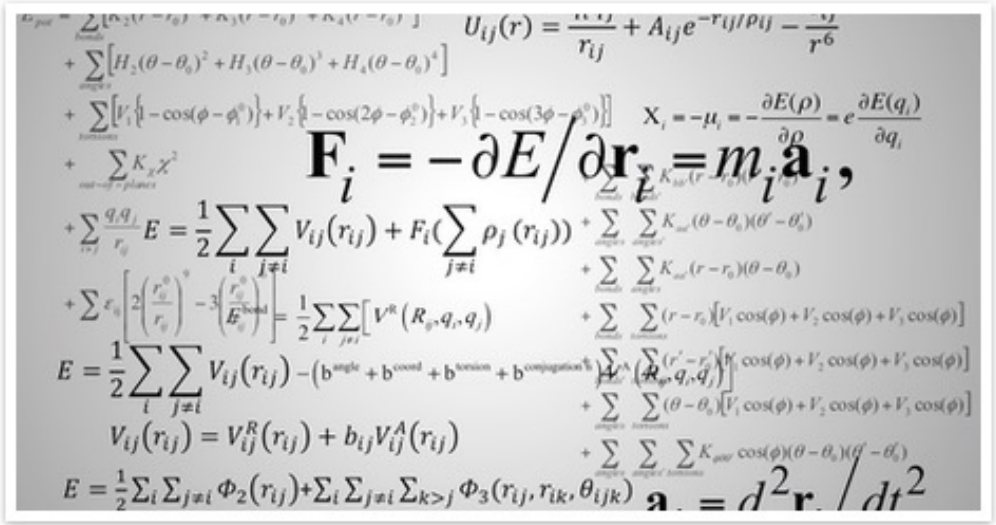
MedeA®-GIBBS simulations (various FFs)

Repeating and extending previous work by:
J. Perez-Pellitero et al., J. Phys. Chem. B 112, p. 9853-9863 (2008)

Past Webinar on MedeA Forcefields

- https://www.materialsdesign.com/webinars/recorded/Classical-Forcefields-for-Modeling-Materials-on-Atomic-Scale

Classical Forcefields for Modeling Materials on Atomic Scale



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Related Resources

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Past Webinar on MedeA LAMMPS

- https://www.materialsdesign.com/webinars/recorded/Harness-the-Power-of-LAMMPS-Molecular-Dynamics-Code-with-MedeA

Harness the Power of LAMMPS Molecular Dynamics Code with MedeA

Watch

Related Resources

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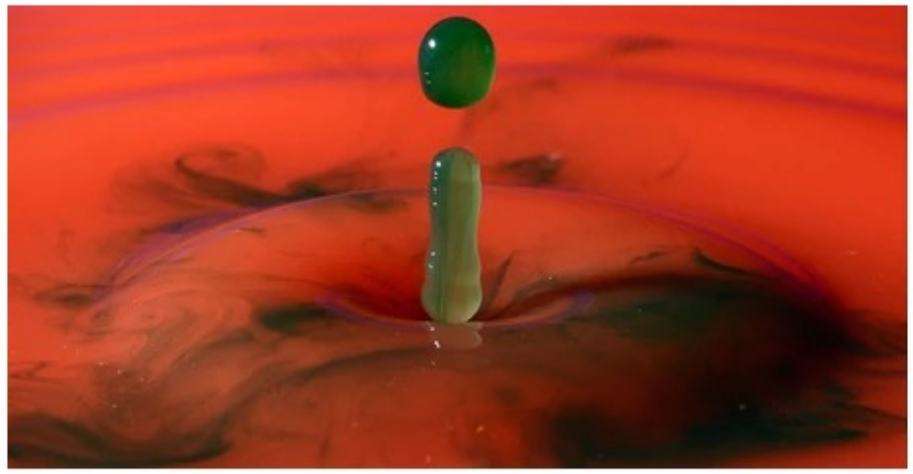
Past Webinar on Fluid Properties

- https://www.materialsdesign.com/webinars/recorded/Fluid-Properties-from-Molecular-Simulation%3A-Applications-in-Chemical-Engineering-and-the-Oil-%26-Gas-Ind

Fluid Properties from Molecular Simulation: Applications in Chemical Engineering and the Oil & Gas Industry



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Past Webinar on Gas Removal

- https://www.materialsdesign.com/webinars/recorded/acid-gas-removal-2021

Molecular Simulations for Improved Process Modeling of an Acid Gas Removal Unit

Watch

Related Resources

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Classical Forcefield-based Methods:

MedeA Mesoscale Capabilities

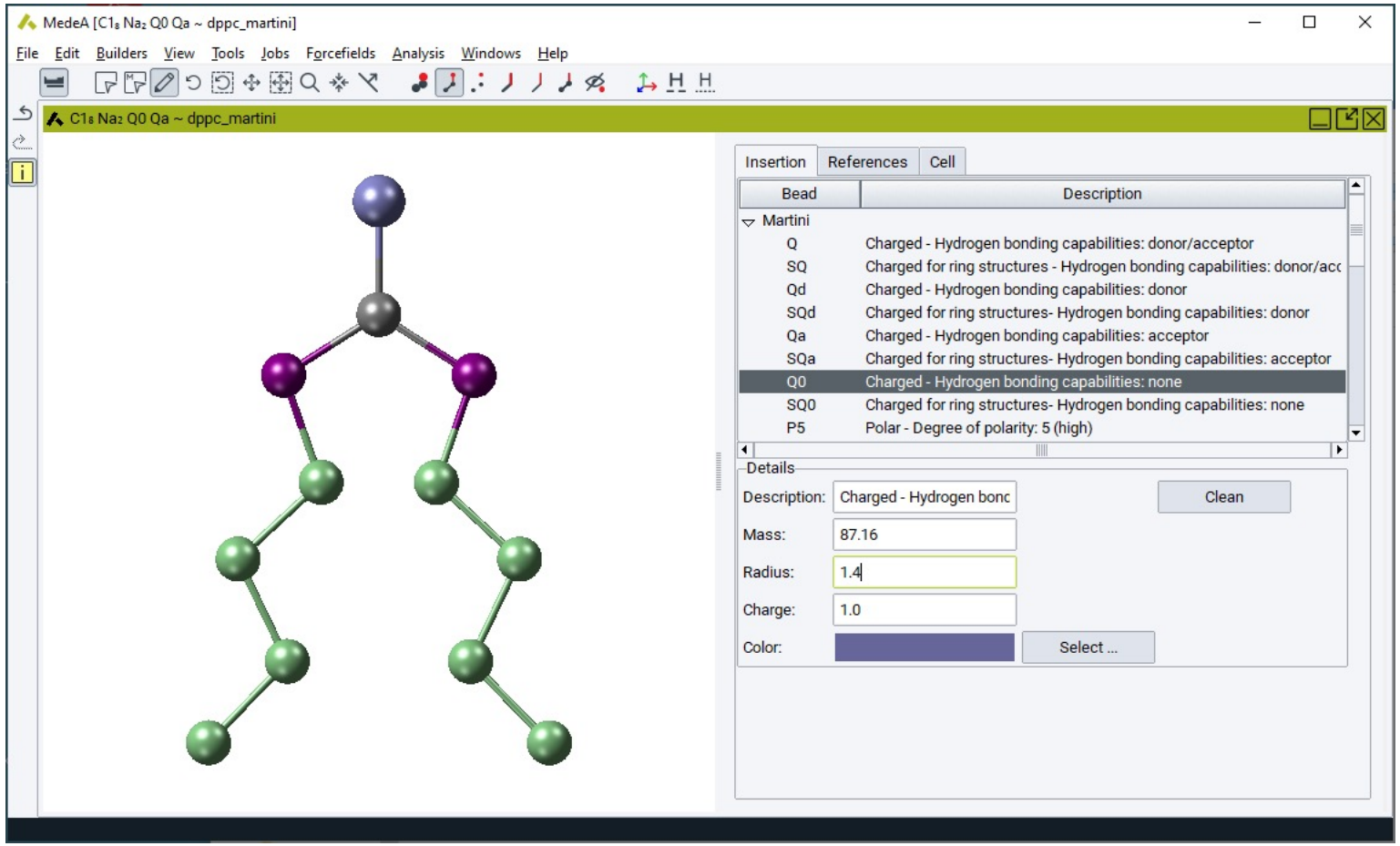
Jörg-Rüdiger Hill

Materials Design

Oct 12, 2021

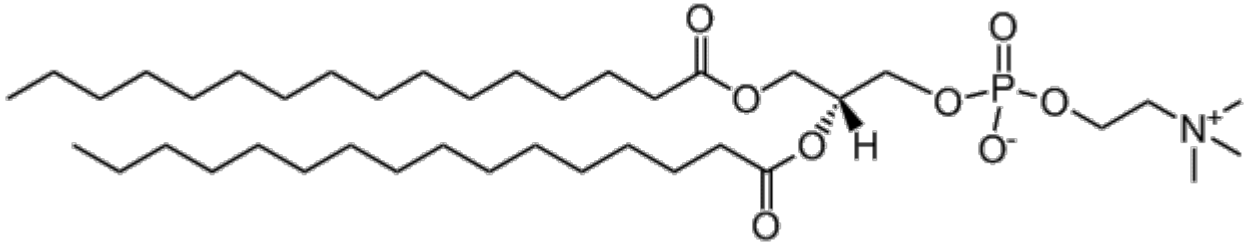
Mesoscale Simulations with *MedeA* 3.3

- *MedeA* 3.3 can be used to create and simulate coarse-grained (mesoscale) systems
- Coarse-grained systems can be used in **polymer builder**, **amorphous builder** and **thermoset builder**
- Simulations can be performed with **LAMMPS** and **GIBBS**, properties can be predicted as for atomistic systems
- Mesoscale simulations can be performed on **microseconds** and **tens of nanometers**



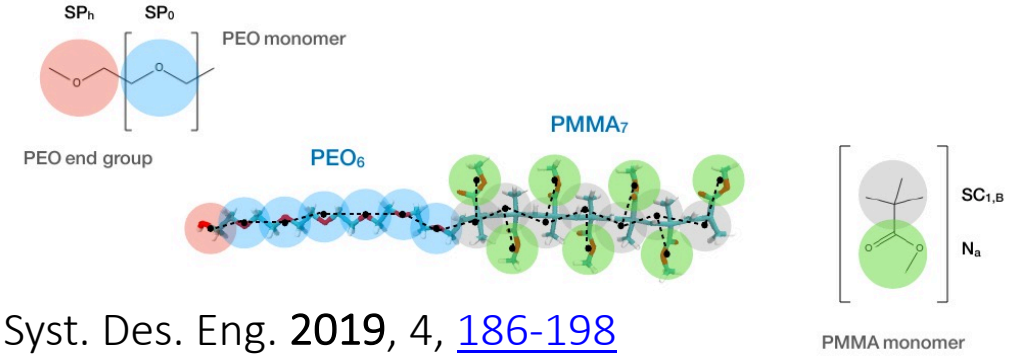
Mesoscale Simulations with *MedeA* 3.3

- Self-assembly of a lipid bilayer
  - Self-assembly of dipalmitoylphosphatidylcholine in water with the Martini forcefield
  - 128 DPPC lipid and 4800 coarse-grained water molecules randomly distributed, 250 ns simulation time



S. J. Marrink, A. H. de Vries, A. E. Mark, J. Phys. Chem. B (2004), 108, 750-760; S. J. Marrink, H. J. Risselada, S. Yefimov, D. P. Tieleman, A. H. de Vries, J. Phys. Chem. B (2007), 111, 7812-7824

- Forward mapping of Poly(ethylene oxide-b-methylmethacrylate)
  - Convert atomistic model to mesoscale model



G. Campos-Villalobos, F. R. Siperstein and A. Patti, Mol. Syst. Des. Eng. **2019**, 4, 186-198

Announcements

Professor Chris Van de Walle

University of California, Santa Barbara

Thursday, October 14th

Thursday, October 14th

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Dr. Erich Wimmer

Materials Design

Professor Chris Van de Walle

University of California, Santa Barbara

Wednesday, October 20th

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Professor Georg Kresse

University of Wien

Dr. René Windiks

Materials Design

Upcoming Plenary Speaker

October 20th

Corresponding Training

October 26th

Questions on Materials Design UGM Trainings

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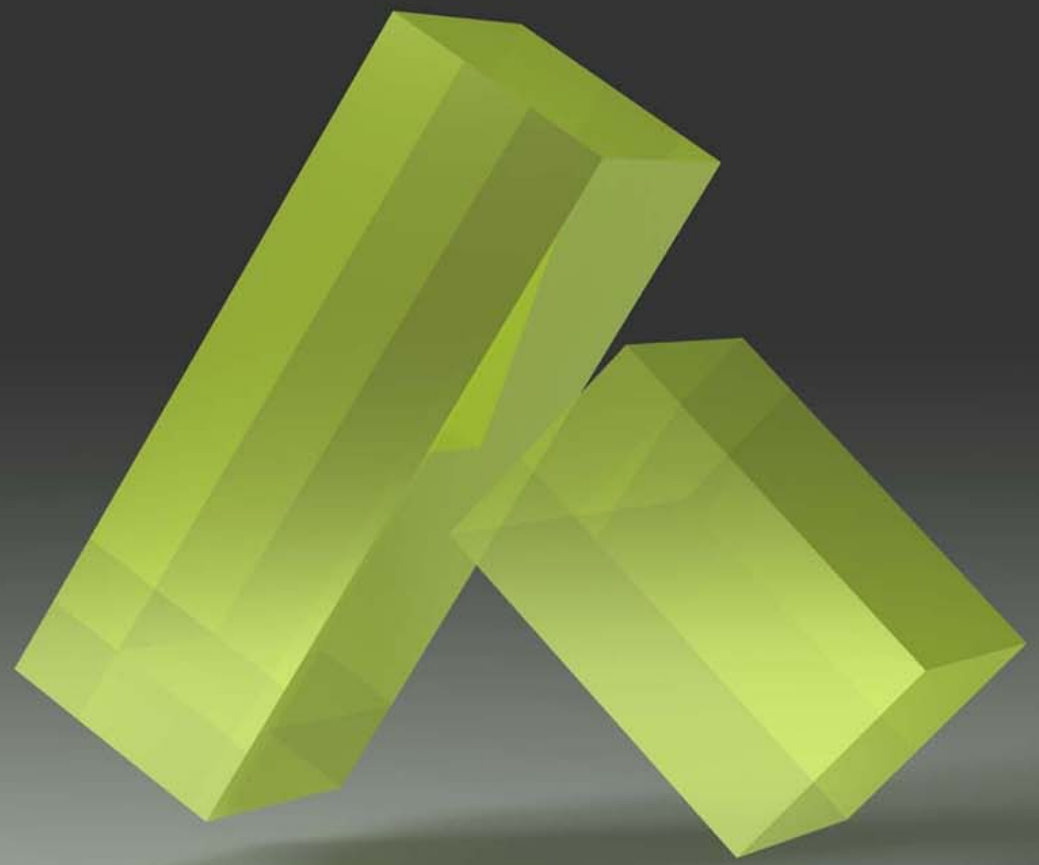
Question and Answer Session

Dr. Marianna Yiannourakou

Dr. Jörg-Rütiger Hill

Dr. Ray Shan



MedeA

Innovation by Simulation