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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

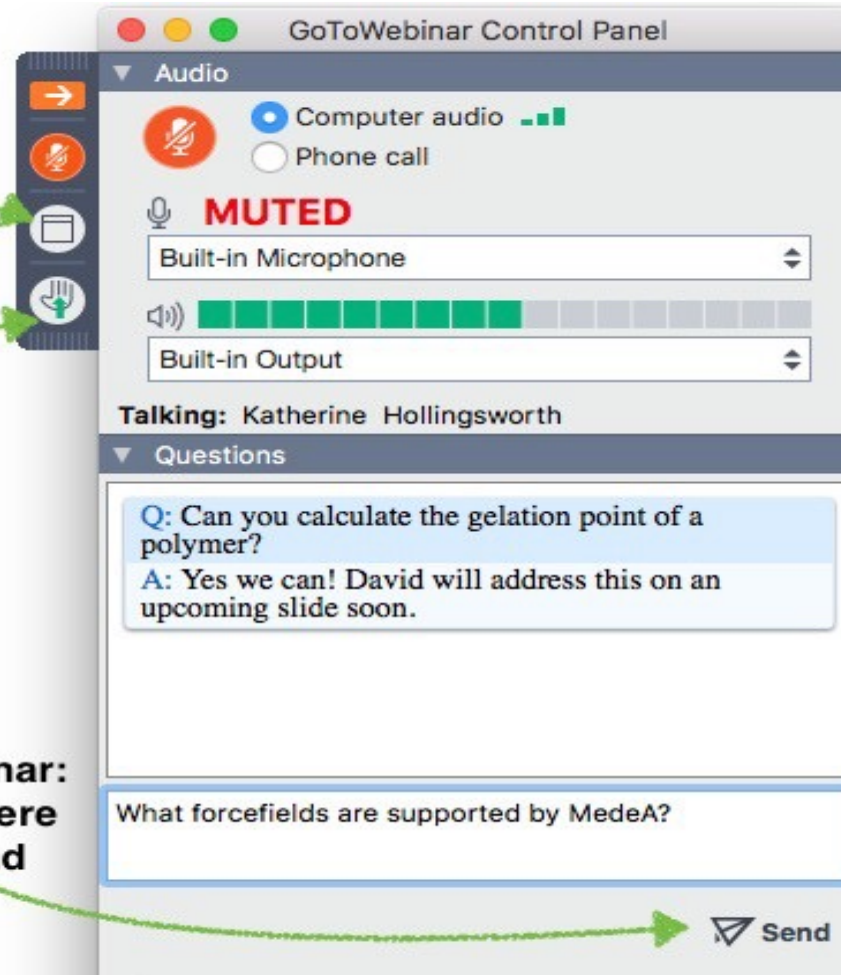
- ▶ Tuesdays in this UGM series will feature online training sessions with members of the Materials Design Team
- ▶ Share the training sessions with your colleagues!
 - Registration details
 - <https://ugm.materialsdesign.com>
- ▶ We will be recording this session
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- ▶ Audio issues
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Please Ask Questions!

Use the raise hand icon to bring attention to your question

full screen
during discussion:

**any time during webinar:
type your question here
and then press Send**



The screenshot shows the GoToWebinar Control Panel interface. It features a sidebar on the left with icons for full screen, mute, and raise hand. The main panel is divided into sections: Audio, Talking, and Questions. The Audio section shows 'Computer audio' selected and the microphone is 'MUTED'. The Talking section shows 'Talking: Katherine Hollingsworth'. The Questions section contains a question and answer: 'Q: Can you calculate the gelation point of a polymer?' and 'A: Yes we can! David will address this on an upcoming slide soon.' Below this is a text input field with the question 'What forcefields are supported by MedeA?' and a 'Send' button.



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

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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.

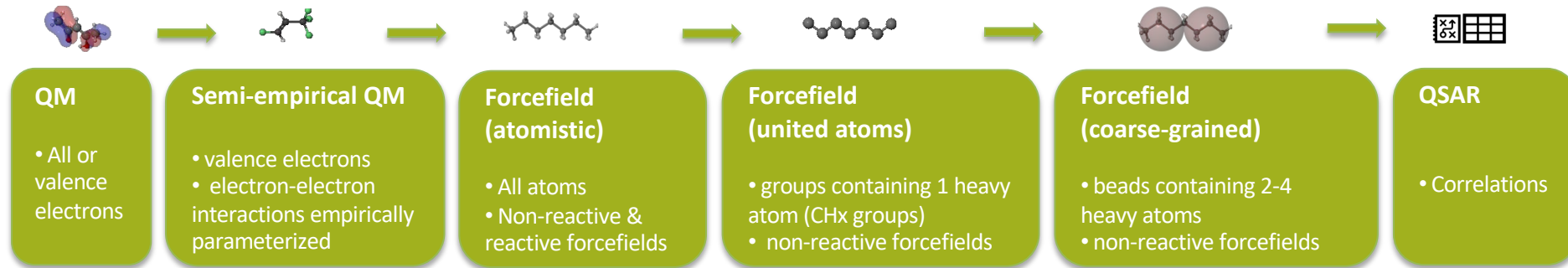
Ungerer, P. ; Tavitian, B. ; Boutin, A. *Applications of Molecular Simulation in the Oil and Gas Industry : Monte Carlo Methods*, Editions Technip - IFP Publications, Paris, France, 2005.



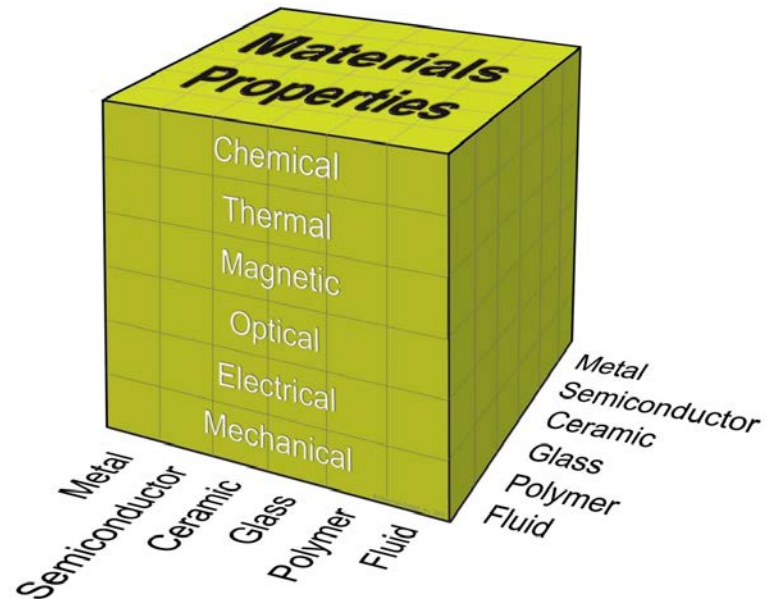
Short overview of Forcefield simulations



Levels of description / Access to information



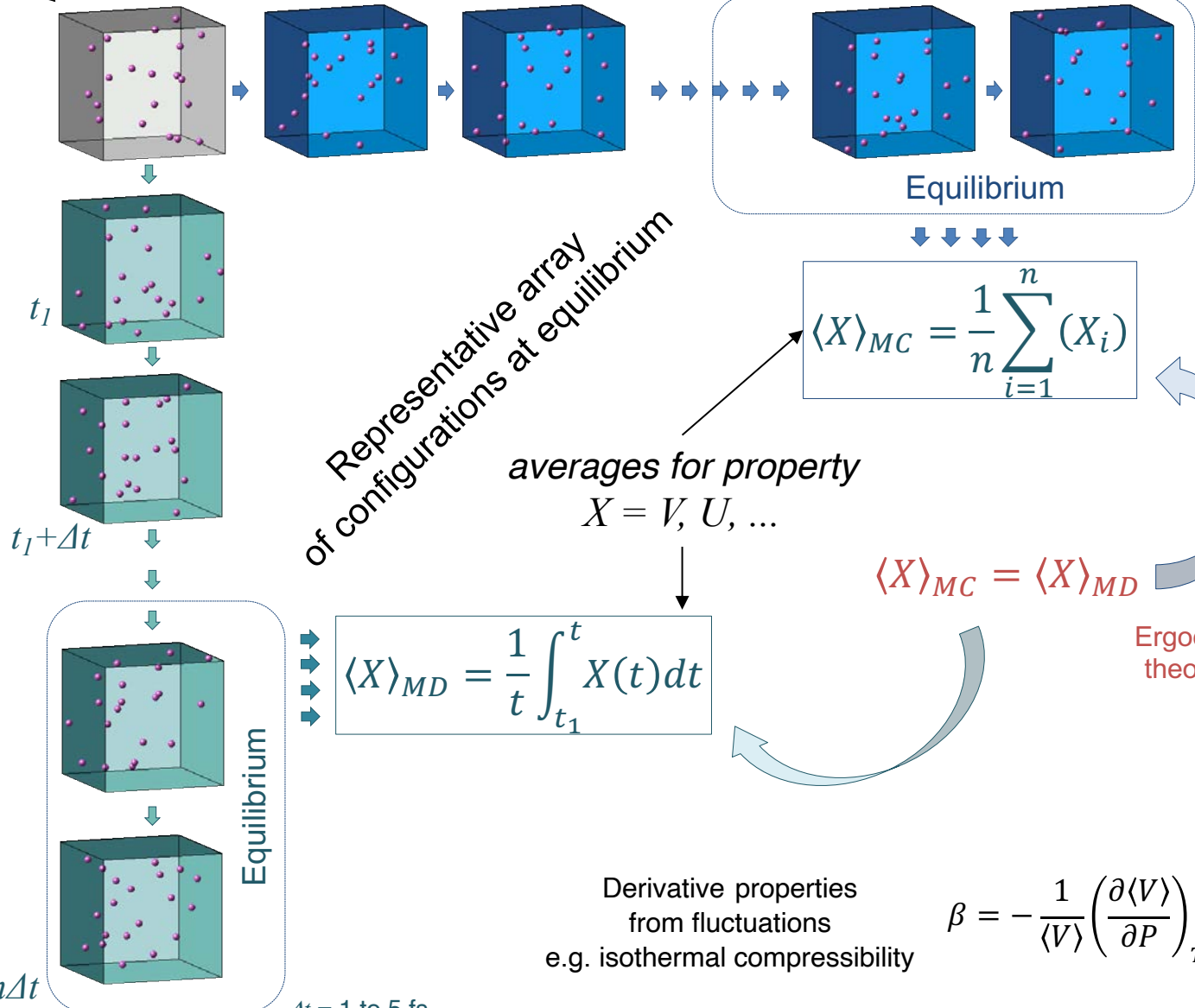
Prediction of materials properties of engineering value



Initial Configuration

Monte Carlo Statistical method (Markov chain & Metropolis)

Molecular Dynamics Integration of Newton's Equations of Motion





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)



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MedeA Forcefields

In *MedeA*, forcefields are the basis for many atomistic simulations. Forcefields allow simulators to study systems with thousands of atoms and over many configurations. For dynamical properties like diffusion, viscosity, and thermal conductivity; or for significant configurational sampling in evaluating sorption or mechanical properties, simulations are based on a forcefield.

In all cases, *MedeA* provides open access to forcefield parameters, and all supporting information, such as atom assignment rules. For any simulation, it is straightforward to access the parameters that were employed in that particular calculation, making it easy to document, assess, and reproduce calculation results.

MedeA Forcefields Bundle

MedeA provides substantial forcefield support by default. For organic systems, *MedeA* supports the most well-established, all-atom PCFF+ forcefield which provides materials properties with the highest accuracy. *MedeA* also support united atom AUA+ and TraPPE-UA+ forcefields. These three forcefields are being actively developed and extended by Materials Design. Additionally, *MedeA* supports COMPASS and OPLS-AA forcefields.

For metallic systems, *MedeA* supports embedded atom method (EAM) forcefields and modified EAM (MEAM) forcefields, and for inorganic systems *MedeA* supports Buckingham, Clay-FF, and variable-charge Streitz-Mintmire forcefields.

For semiconductor systems, Tersoff and Stillinger-Weber forcefields are supported, and when bond breaking and making is simulated, *MedeA* supports the REBO and variable-charge COMB3 and ReaxFF forcefields.

Occasionally, when opportunities for improvement are identified, forcefield parameters are updated. Materials Design is committed to the development of accurate and validated forcefield parameters.

<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

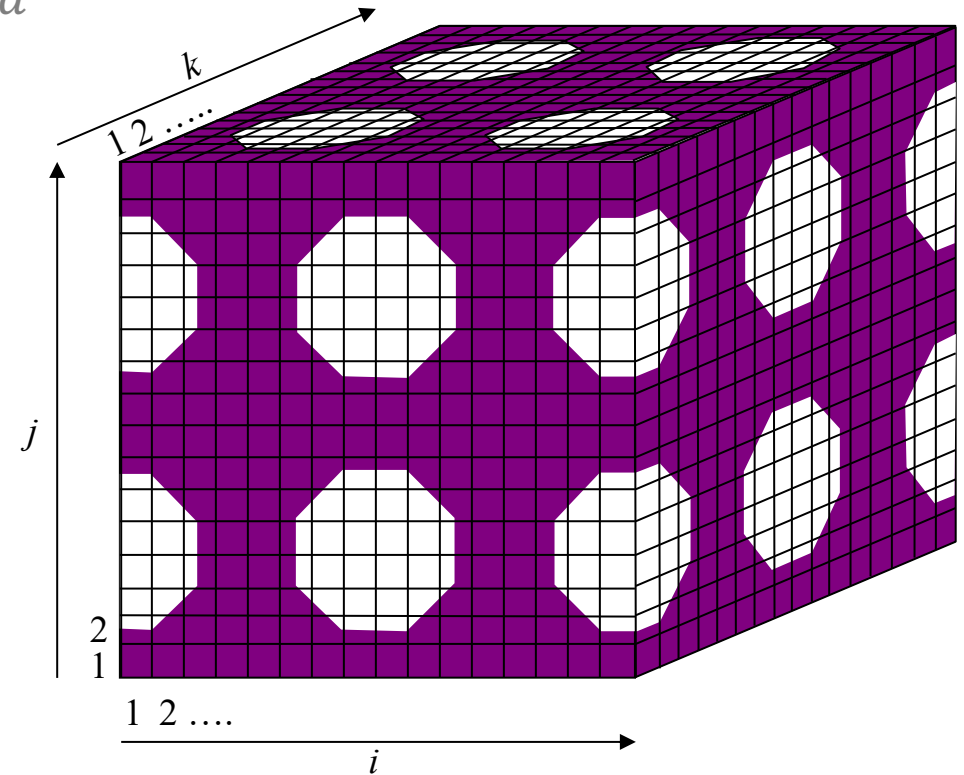


Interaction energy between the molecules and the adsorbent

Neglected (no solid deformation)



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



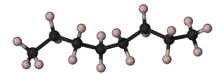


Characterization and Sorption

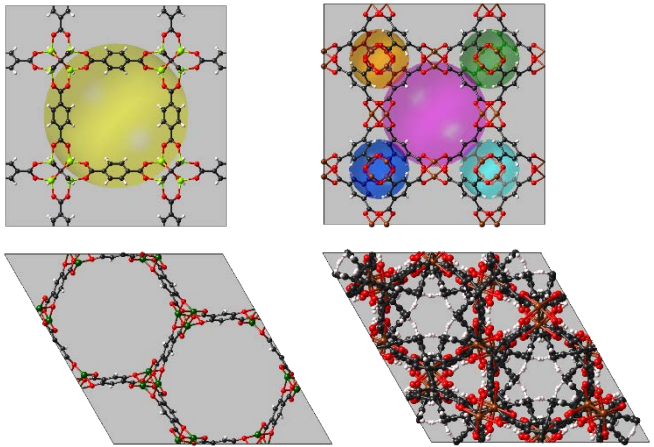
1 Create a system

- 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)

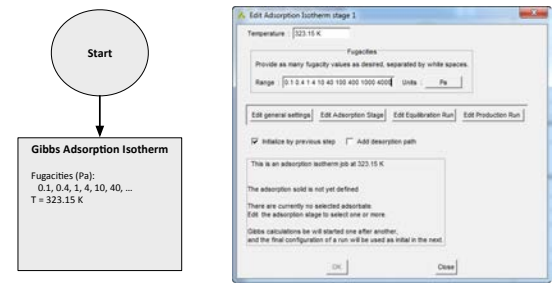
Adsorbate



Adsorbent



2 Run MC simulations to get sorption isotherms



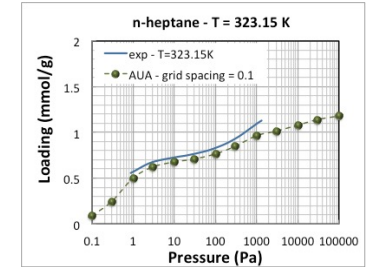
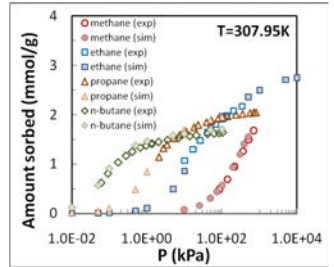
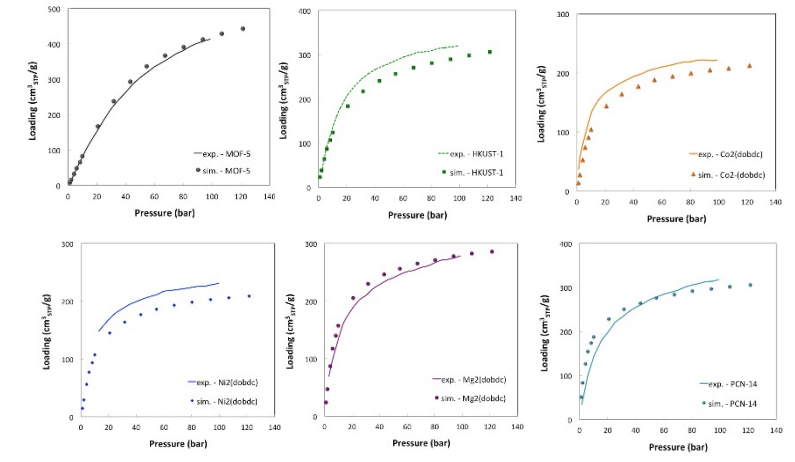
- Submit a single job to get an entire isotherm
- Run adsorption & desorption paths
- Chose to have mobile or immobile cations in a zeolite

3 Get Results

Gibbs stage completed on Thu 03 February 2022 at 12:07:22 EDT after 23h 4 (127116)

Iteration	Temperature (K)	Pressure (bar)	Adsorbed amount (mmol/g)	Desorbed amount (mmol/g)	Specific heat (J/mol-K)	Status
1	323.15	0.1	0.000000	0.000000	24.24	converged
2	323.15	0.1	0.000000	0.000000	24.24	converged
3	323.15	0.1	0.000000	0.000000	24.24	converged
4	323.15	0.1	0.000000	0.000000	24.24	converged
5	323.15	0.1	0.000000	0.000000	24.24	converged
6	323.15	0.1	0.000000	0.000000	24.24	converged
7	323.15	0.1	0.000000	0.000000	24.24	converged
8	323.15	0.1	0.000000	0.000000	24.24	converged
9	323.15	0.1	0.000000	0.000000	24.24	converged
10	323.15	0.1	0.000000	0.000000	24.24	converged
11	323.15	0.1	0.000000	0.000000	24.24	converged
12	323.15	0.1	0.000000	0.000000	24.24	converged
13	323.15	0.1	0.000000	0.000000	24.24	converged
14	323.15	0.1	0.000000	0.000000	24.24	converged
15	323.15	0.1	0.000000	0.000000	24.24	converged
16	323.15	0.1	0.000000	0.000000	24.24	converged
17	323.15	0.1	0.000000	0.000000	24.24	converged
18	323.15	0.1	0.000000	0.000000	24.24	converged
19	323.15	0.1	0.000000	0.000000	24.24	converged
20	323.15	0.1	0.000000	0.000000	24.24	converged

- 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



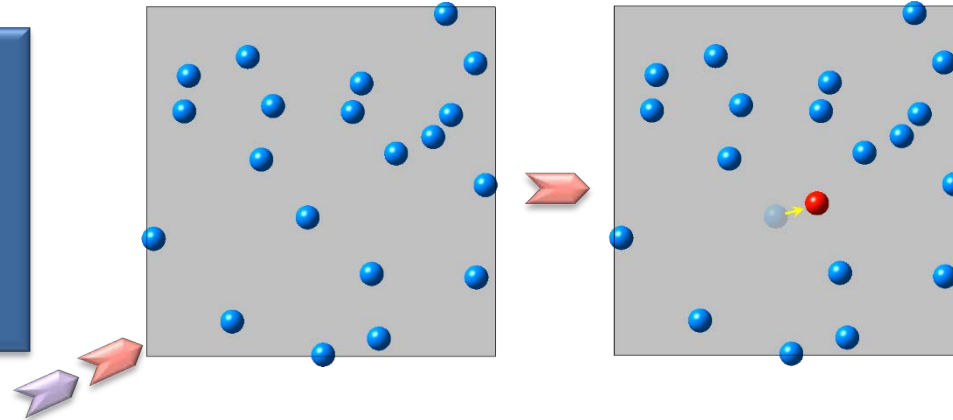
Widom test insertions in the NVT & NPT ensembles

CANONICAL ENSEMBLE: (NVT)

Input / Imposed Quantities:

- N (number of molecules) \rightarrow constant
- V (Volume) \rightarrow constant
- T (Temperature) \rightarrow constant

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

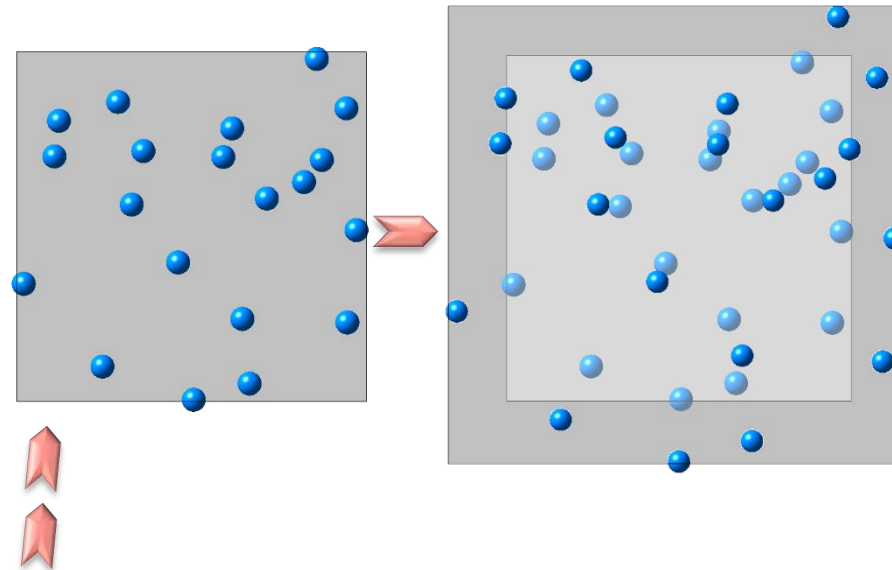


ISOTHERMAL-ISOBARIC ENSEMBLE: (NPT)

Input / Imposed Quantities:

- N (number of molecules) \rightarrow constant
- P (Pressure) \rightarrow constant
- T (Temperature) \rightarrow constant

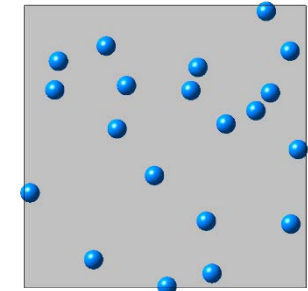
- Translation (atoms & molecules)
- Rotation (molecules)
- Internal moves (flexible molecules)
- Volume change (expansion/ compression)



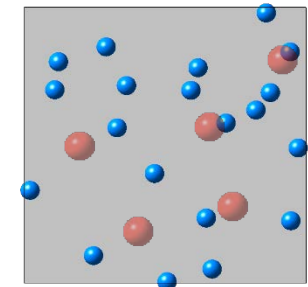
Widom test insertion:

- 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

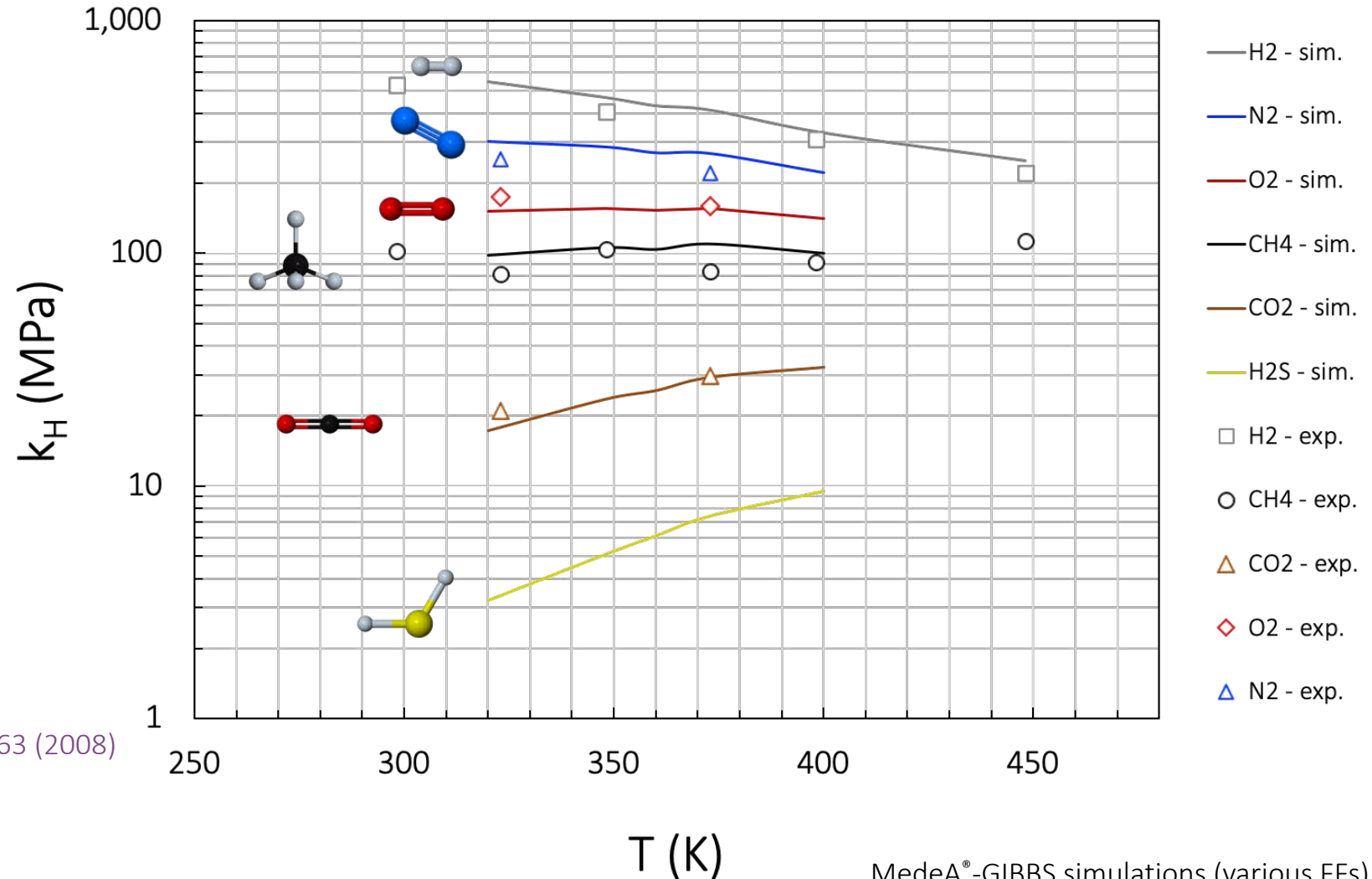
Henry's law: $P_i = K_{H,i} \cdot x_i$

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)

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



MedeA®-GIBBS simulations (various FFs)



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

$$U_{ij}(r) = \frac{A_{ij}}{r_{ij}} + A_{ij}e^{-r_{ij}/\rho_{ij}} - \frac{C_{ij}}{r_{ij}^6}$$

$$+ \sum_{\text{angles}} [H_2(\theta - \theta_0)^2 + H_3(\theta - \theta_0)^3 + H_4(\theta - \theta_0)^4]$$

$$+ \sum_{\text{torsions}} [V_1 \{1 - \cos(\phi - \phi_0)\} + V_2 \{1 - \cos(2\phi - \phi_0)\} + V_3 \{1 - \cos(3\phi - \phi_0)\}]$$

$$+ \sum_{\text{non-bonded planes}} K_{\chi} \chi^2$$

$$+ \sum_{\text{charges}} \frac{q_i q_j}{r_{ij}}$$

$$+ \sum_{\text{dipoles}} \epsilon_i \left[2 \left(\frac{r_{ij}^3}{r_i^3} \right) - 3 \left(\frac{r_{ij}^3}{r_j^3} \right) \right] = \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij}(r_{ij}) + F_i \left(\sum_{j \neq i} \rho_j(r_{ij}) \right) + \sum_{\text{angles}} \sum_{\text{torsions}} K_{\omega} (\theta - \theta_0)(\theta' - \theta'_0)$$

$$+ \sum_{\text{non-bonded}} \sum_{\text{planes}} K_{\omega} (r - r_0)(\theta - \theta_0)$$

$$+ \sum_{\text{charges}} \sum_{\text{dipoles}} (r - r_0) [V_1 \cos(\phi) + V_2 \cos(\phi) + V_3 \cos(\phi)]$$

$$+ \sum_{\text{charges}} \sum_{\text{dipoles}} (\theta - \theta_0) [V_1 \cos(\phi) + V_2 \cos(\phi) + V_3 \cos(\phi)]$$

$$+ \sum_{\text{charges}} \sum_{\text{dipoles}} \sum_{\text{planes}} K_{\text{pov}} \cos(\phi)(\theta - \theta_0)(\theta' - \theta'_0)$$

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij}(r_{ij}) - (b^{\text{angle}} + b^{\text{coord}} + b^{\text{bonds}} + b^{\text{conjugation}}) \sum_{\text{atoms}} \sum_{\text{planes}} \left(\frac{r' - r_0}{r_0} \right)^6 [V_1 \cos(\phi) + V_2 \cos(\phi) + V_3 \cos(\phi)]$$

$$+ \sum_{\text{charges}} \sum_{\text{dipoles}} (\theta - \theta_0) [V_1 \cos(\phi) + V_2 \cos(\phi) + V_3 \cos(\phi)]$$

$$+ \sum_{\text{charges}} \sum_{\text{dipoles}} \sum_{\text{planes}} K_{\text{pov}} \cos(\phi)(\theta - \theta_0)(\theta' - \theta'_0)$$

$$V_{ij}(r_{ij}) = V_{ij}^R(r_{ij}) + b_{ij} V_{ij}^A(r_{ij})$$

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} \Phi_2(r_{ij}) + \sum_i \sum_{j \neq i} \sum_{k > j} \Phi_3(r_{ij}, r_{ik}, \theta_{ijk}) \quad \mathbf{a} = d^2 \mathbf{r} / dt^2$$

Watch

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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



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Related Resources

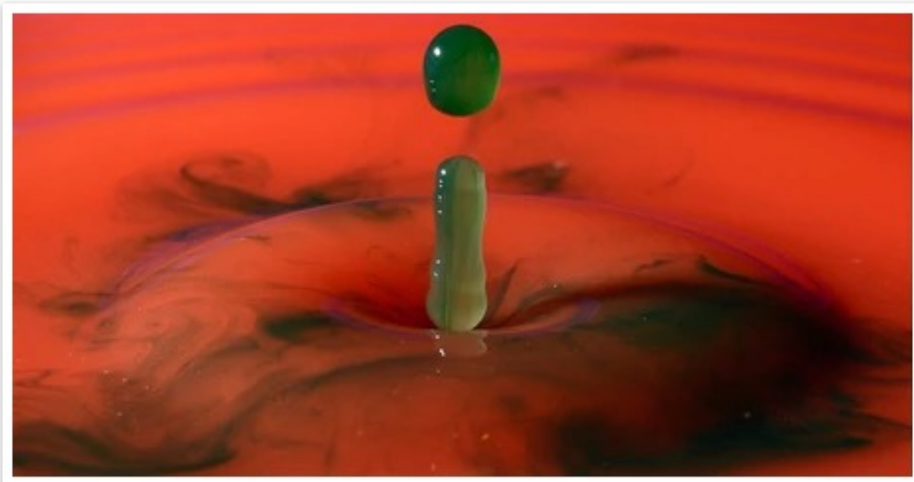
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Past Webinar on Fluid Properties

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

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



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Classical Forcefield-based Methods: MedeA Mesoscale Capabilities

Jörg-Rüdiger Hill
Materials Design

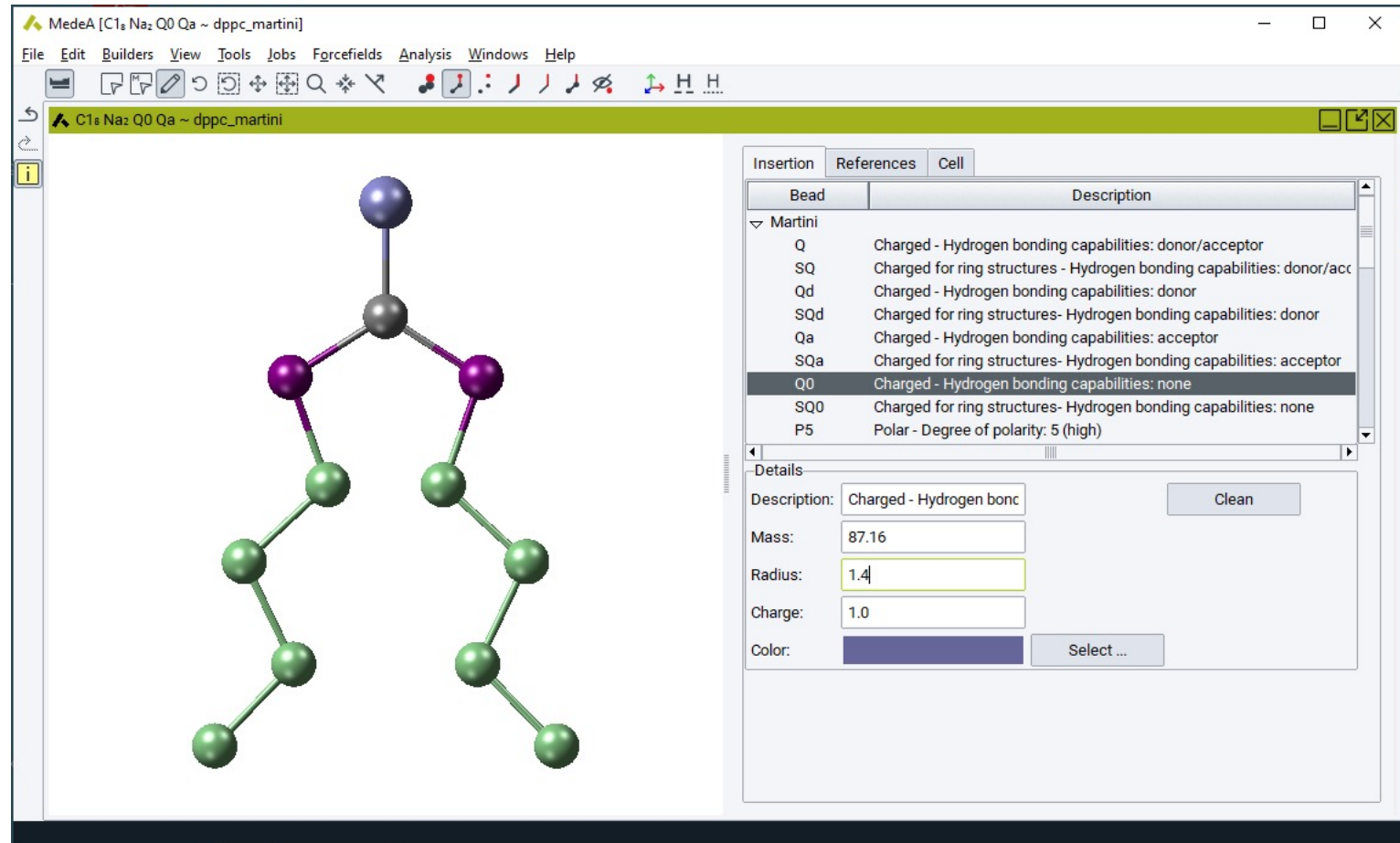
Oct 12, 2021

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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**

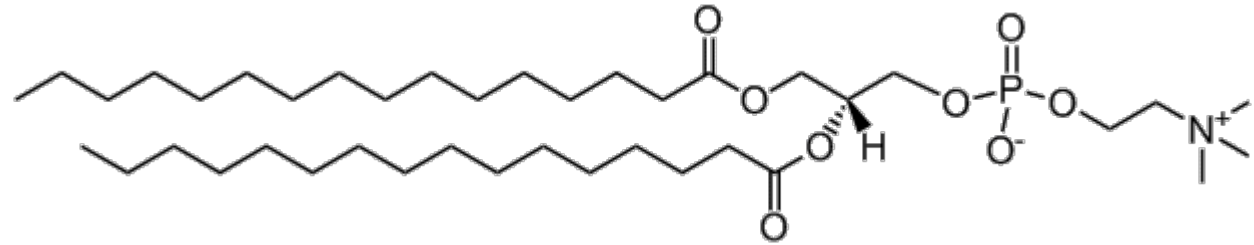




Mesoscale Simulations with *MedeA* 3.3

► Self-assembly of a lipid bilayer

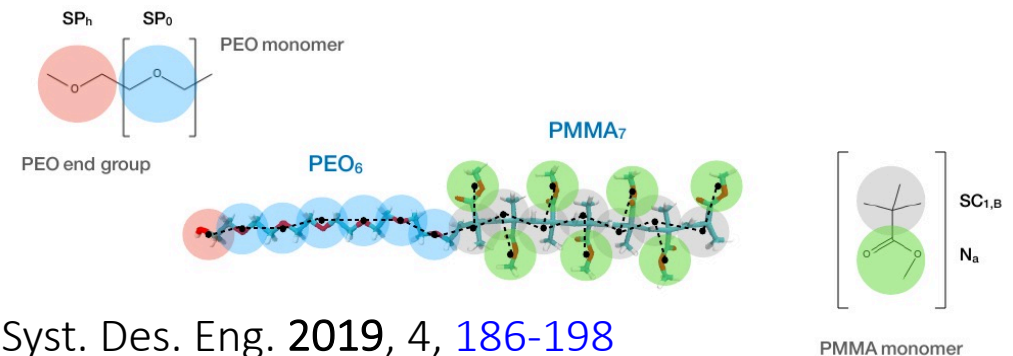
- Self-assembly of dipalmitoylphosphatidylcholine in water with the Martini forcefield
- 128 DPPC lipid and 4800 coarse-grained water molecules randomly distributed, 250 ns simulation time



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

Upcoming Plenary Speaker

October 20th



Dr. René Windiks

Materials Design

Corresponding Training

October 26th

Questions on Materials Design UGM Trainings

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info@materialsdesign.com

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Question and Answer Session



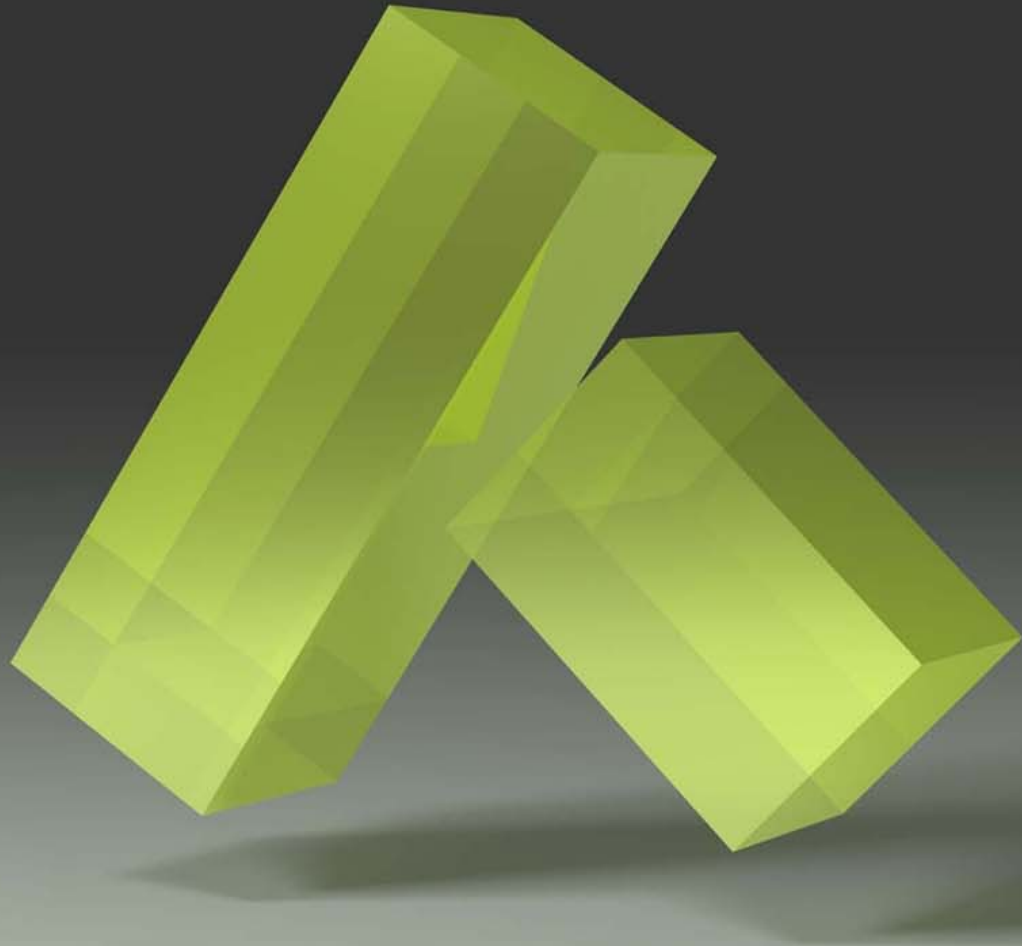
Dr. Marianna Yiannourakou



Dr. Jörg-Rütiger Hill



Dr. Ray Shan



Medea

Innovation by Simulation