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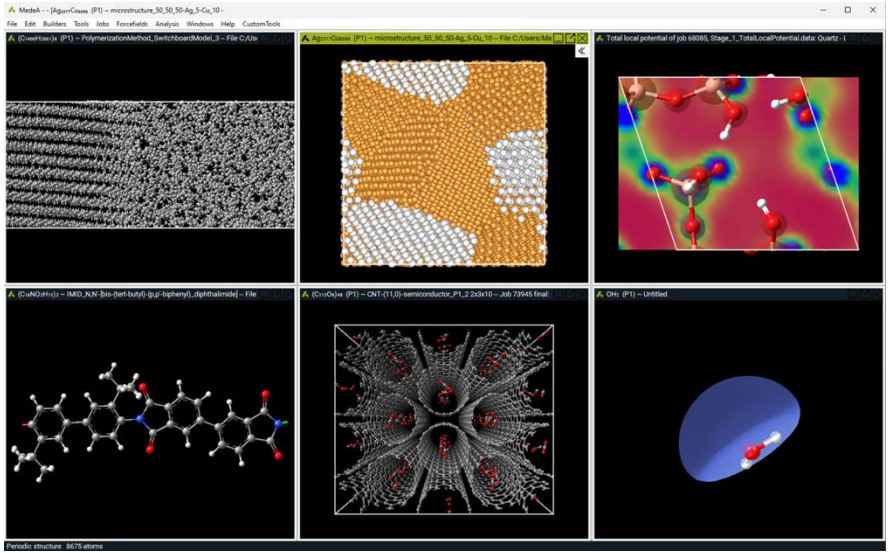
High-Throughput Molecular Simulations for Gas Sorption in Polymers: Automated Workflows for Industrial Material Design



Marianna Yiannourakou & Dave Rigby

24 February 2026

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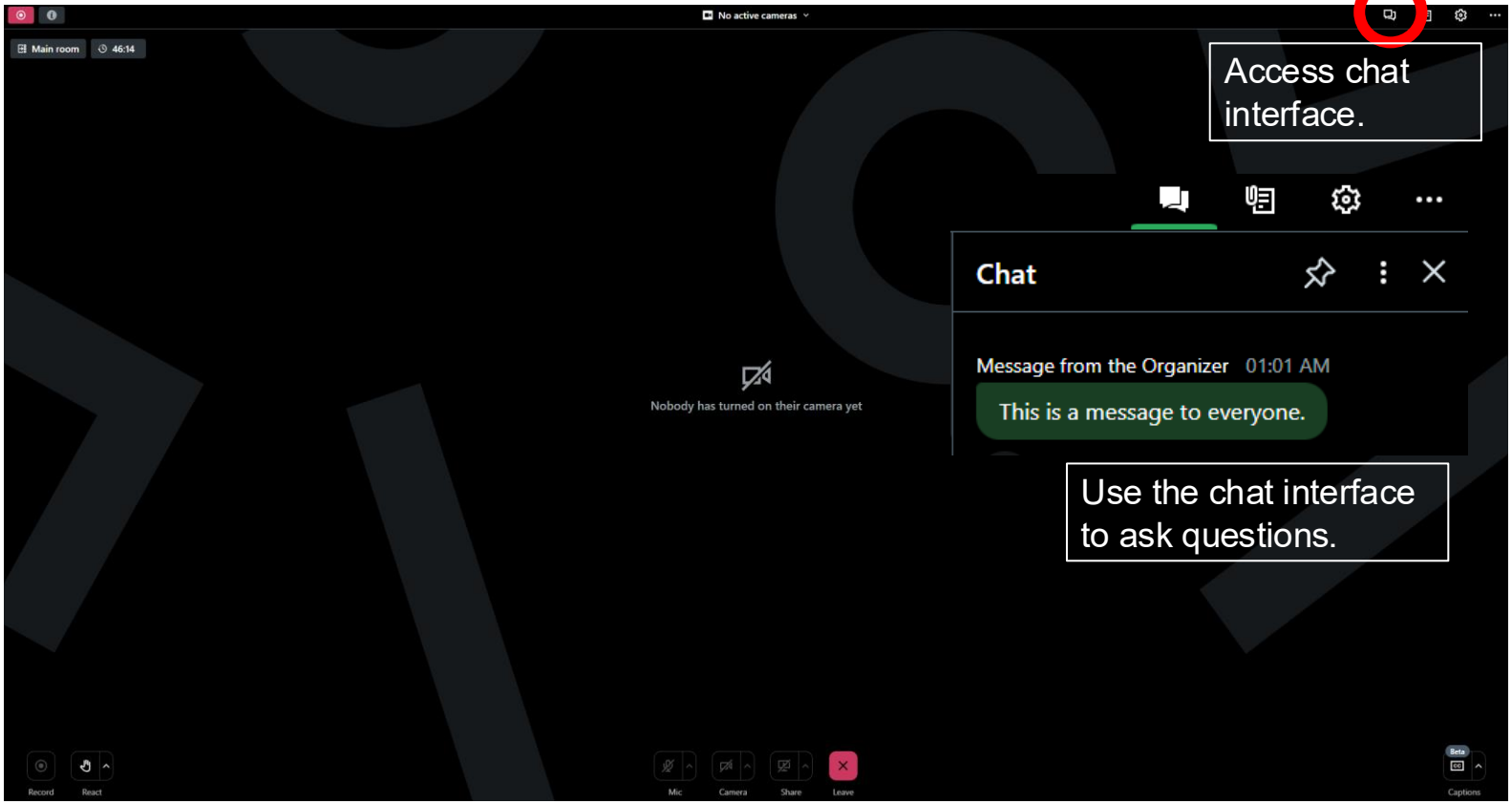

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Webinar Speakers

Katherine Hollingsworth *Dr. Marianna Yiannourakou* *Dr. David Rigby* *Dr. Benoit Minisini*

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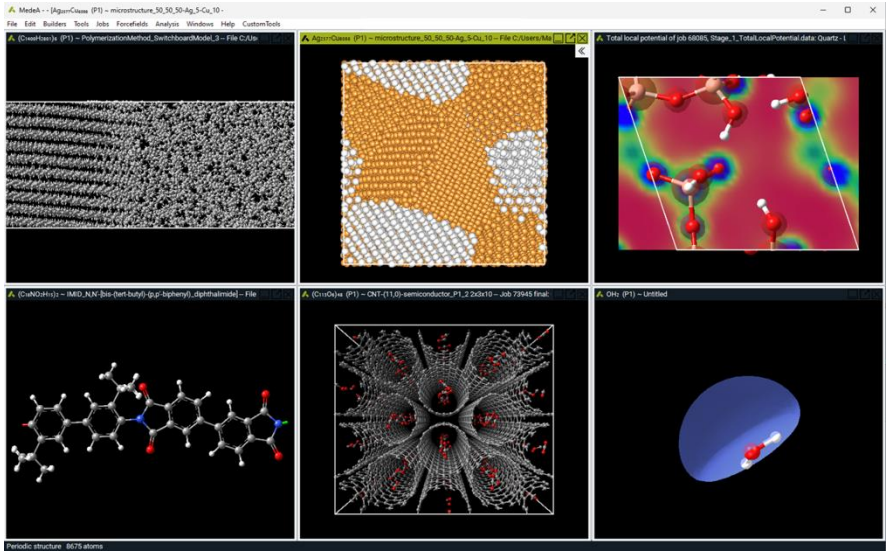
High-Throughput Molecular Simulations for Gas Sorption in Polymers: Automated Workflows for Industrial Material Design



Marianna Yiannourakou & Dave Rigby

24 February 2026

Polymers: High & Low Tech Materials

- Polymers are encountered in a wide variety of applications, in:
  - Aerospace:
    - Advanced high temperature composite matrices
    - Vehicle re-entry heat shields
  - Electronics:
    - Flexible displays, conducting polymers, printed circuit boards, photoresists, and packaging/molding compounds
  - Membranes:
    - Fuel cells, water purification, gas separation
  - Textiles and fibers
  - Adhesives and Coatings
  - Foods (e.g. polysaccharides)
  - Living organisms:
    - Cell membranes (polysaccharides, lipids, proteins)

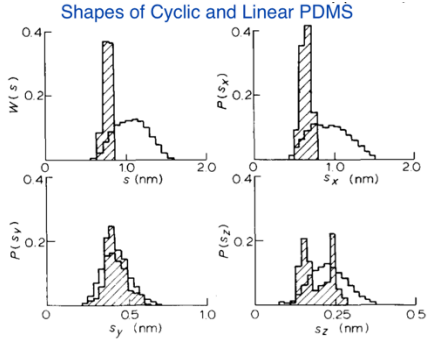
Modeling Opportunities

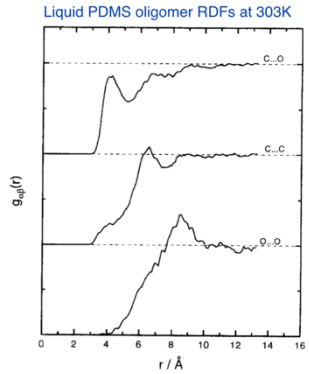
- Polymeric materials research opportunities
  - Diagnosis of failure mechanisms
  - Improved performance and efficiency (e.g. higher strength, increased service life, …)
  - Cost reduction
  - Development of alternative materials
    - Environmental regulation
    - Avoiding conflict with patents
  - Designing new materials prior to synthesis or fabrication

- Some advantages of polymer modeling
  - Predicting behavior in hostile environments
  - Reducing the need for expensive experiments
  - Detailed molecular level understanding of material behavior

Need for High Throughput Modeling

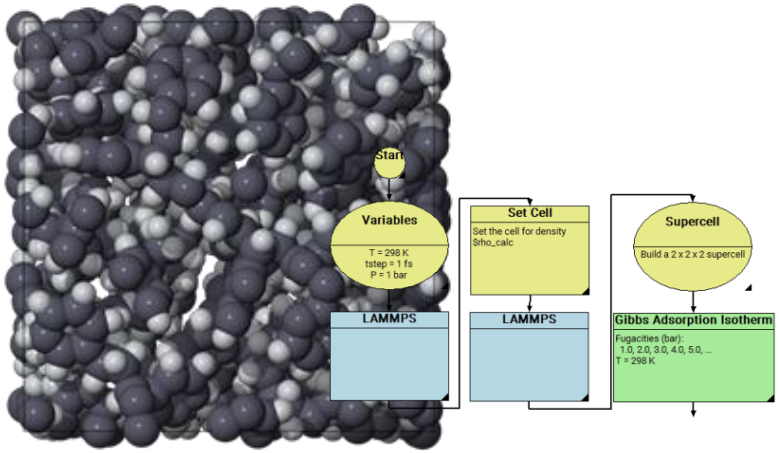
1. Polymer chains invariably exhibit broad distributions of spatial configurations.
2. In addition, the disordered amorphous, liquid-like packing of polymers in the bulk leads to a range of intermolecular distances even at short range





3. The net result is that averaging computed properties over many polymer configurations is almost always essential when working with polymers…

Permeability of O_2 in atactic polystyrene (PS)



Permeation and Permeability

Permeation is usually described experimentally by a **permeability coefficient**, *P*, defined by[1]:

$$P = \frac{(quantity\ of\ permeant) \times (membrane\ thickness)}{(area) \times (time) \times (pressure\ drop\ across\ membrane)}$$

which is equivalent to the following:

$$P = D \times S$$

where *D* denotes the diffusivity, and *S* the solubility.

In atomistic simulations of gas penetrant systems, *D* can often be obtained directly using molecular dynamics simulation, while *S* can be obtained by Monte Carlo methods.

1. see, for example, Polymer Handbook, J. Brandrup & E.H. Immergut (eds)

Permeability coefficient of O_2 in atactic polystyrene (PS)

Schematic representation of the Permeability calculation:

System building (MedeA Polymer Builder, MedeA Amorphous Builder) → Solubility calculation (MedeA GIBBS) → Diffusivity calculation (MedeA LAMMPS) → Automation and Analysis

System Studied

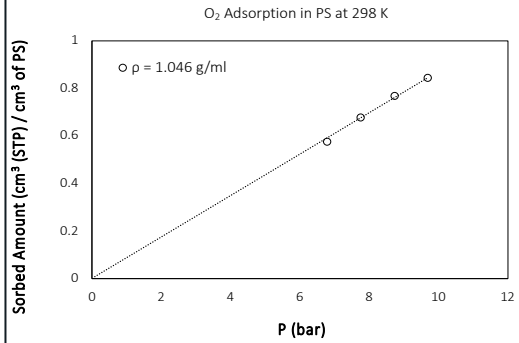
Model system containing 2 atactic PS molecules with DP=80

Pressure dependence of solubility of O_2 in atactic PS at 298K

- $S = \frac{C_{O_2}}{P_{O_2}}$

where O_2 is the concentration of the gas in the polymer and, P_{O_2} is the pressure of the gas

- ***S = 0.872 10⁻⁶ cm³ (STP) / cm³ of PS / Pa***

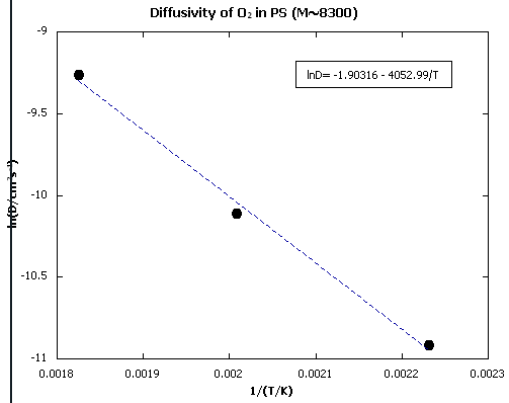


Note: 0.85 cm³(STP)/cm³ of PS corresponds to ~2.4 molecules per simulation box

Arrhenius plot for O_2 in atactic PS (548K-448K)

Model system containing 2 atactic PS molecules with DP=80 and 8 O_2 molecules

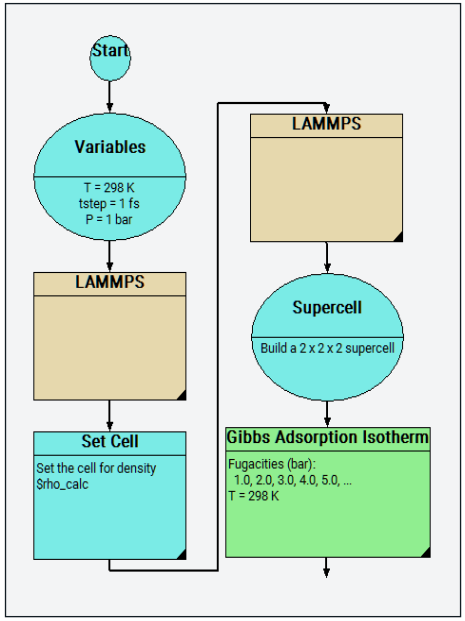
- D ~ **1.87 x 10⁻⁷ cm²s⁻¹ at 298K**

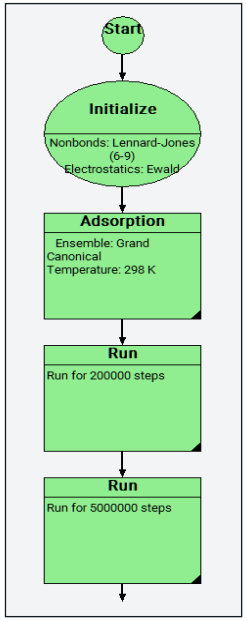


4.1. Permeability coefficient of O_2 in atactic polystyrene (PS)

Schematic representation of the Permeability calculation:

System building (MedeA Polymer Builder, MedeA Amorphous Builder) → Solubility calculation (MedeA GIBBS) → Diffusivity calculation (MedeA LAMMPS) → Automation and Analysis





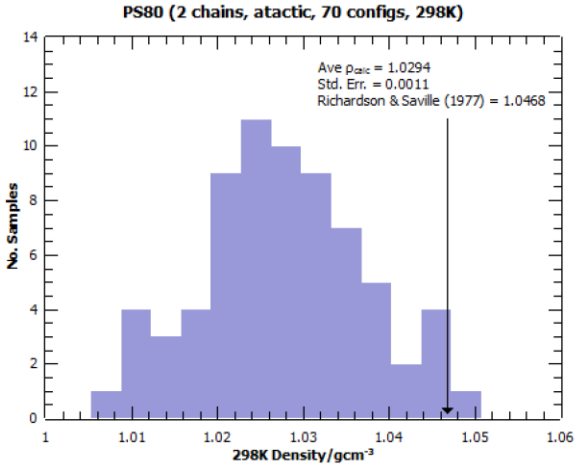
Comparison of calculated and experimental permeability data for O_2 in atactic PS at 298K

	D ($x10^7$)[a] [cm^2/s]	S ($x10^6$)[b] [$cm^3(STP)/(cm^3.Pa$]	P ($x10^{13}$)[c] [$cm^3(STP).cm/(cm^2.s.Pa)$]
Calculated	**1.87**	**0.87**	**1.63**
Burmeister et al	-	-	1.35-1.85
Wang & Ogilby	2.0+0.2	-	-
Rharbi et al	1.9+0.05	-	1.71-1.89

References:
Burmeister et al, Polym. Prepr. ACS Div Polym. Chem. **27**, 414 (1986)
Wang & Ogilby, Can. J. Chem. **73**, 1831 (1995)
Rharbi et al., Anal. Chem. **71**, 5045 (1999)

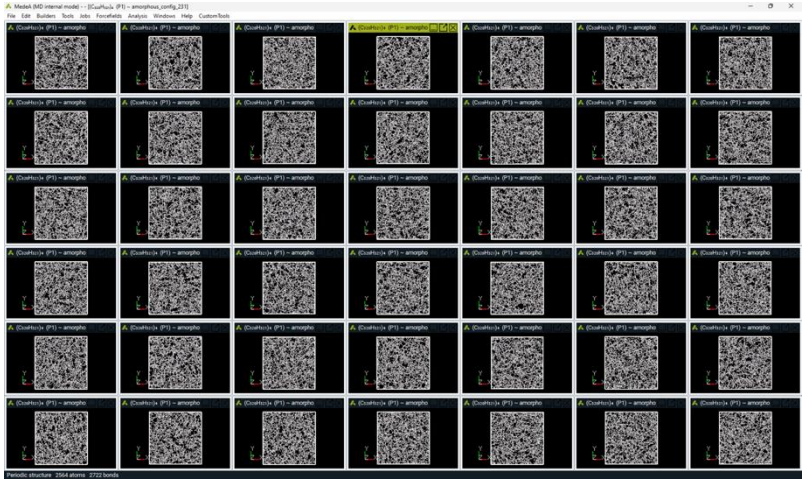
Building multiple models

- Sampling is crucial for determining the sensitivity of the method and the expected accuracy
- Multiple simulation jobs starting from independent initial configurations are required to allow for the accurate calculation of the desired properties

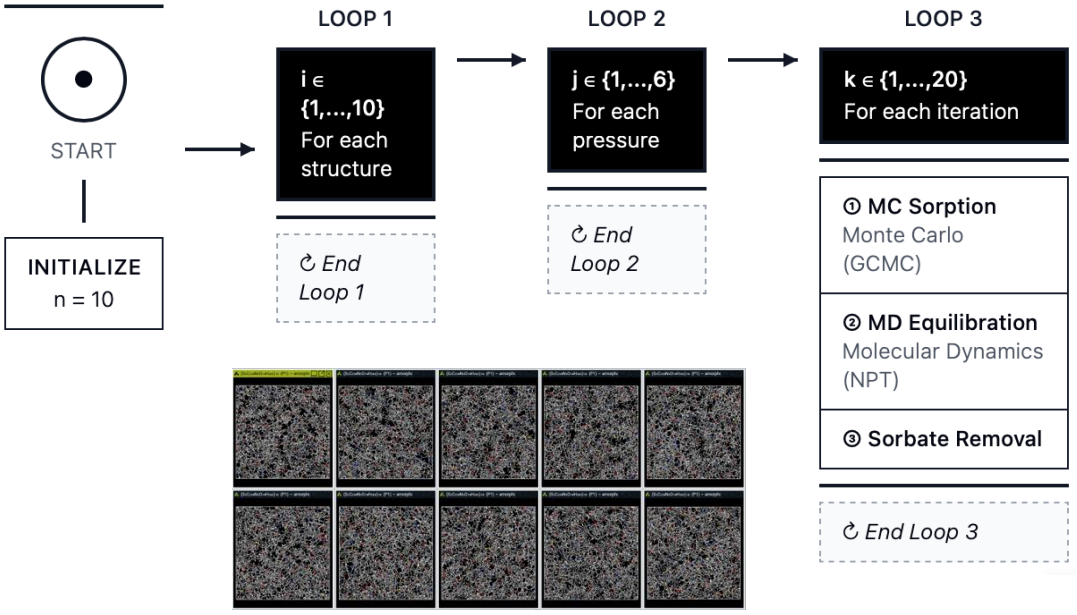


PS80 (2 chains, atactic)

Many realistic initial models are required for appropriate sampling of configuration space and efficient property prediction

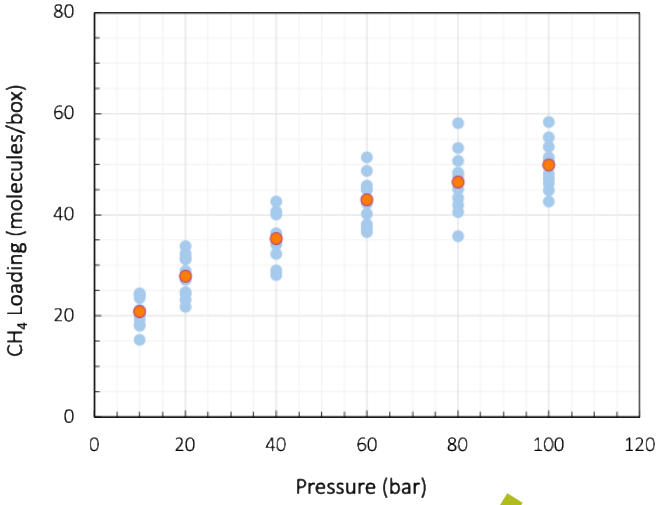


Simulation Workflow

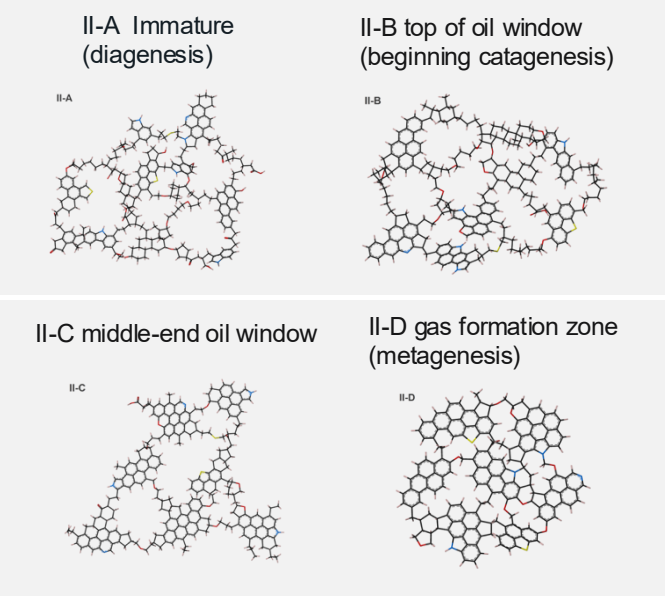


COMPUTATIONAL SUMMARY

Structures		Pressures		Iterations		Total Simulations
10	×	6	×	20	=	1,200



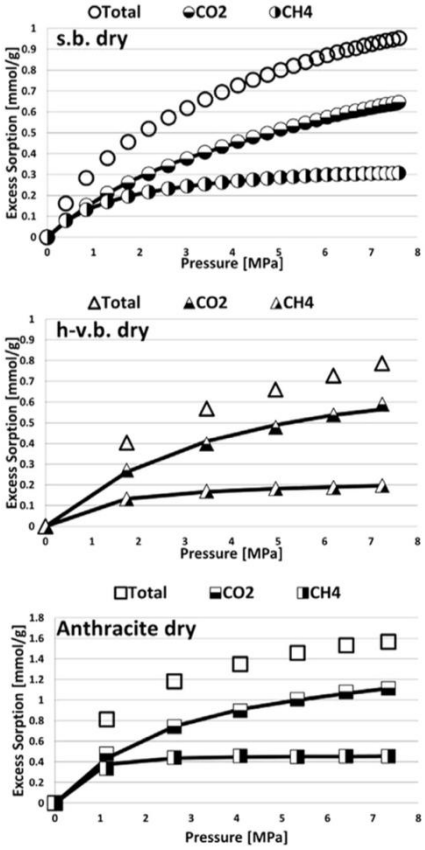
Sorption of CH_4 / CO_2 in kerogen, with swelling



Kerogen models available at:
https://www.materialsdesign.com/Publications/Ungerer2015

Sorption of mixtures of CH_4/CO_2 in dry and moist coal samples

- Merkel et al. (2015) have studied the competitive sorption of CH_4, CO_2 and H_2O on natural coals of different rank
- The feed composition used was rich in methane (70-85%)
- CO_2 is preferably sorbed over CH_4 for dry and moist samples
- CO_2 selectivity over CH_4 tends to decrease with increasing maturity and moisture content
- The mean selectivity for the 3 investigated coals varies between 6 and 9
- The total gas (CH_4 & CO_2) excess sorption capacity is reduced when there is moisture in the coal sample (most pronounced for the subbituminous coal)
- Anthracite presents the highest sorption capacity for dry and moist samples



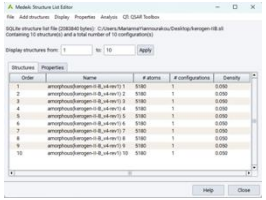
Merkel et al., Int. J. Coal Geology 150-151, p. 181-192 (2015)

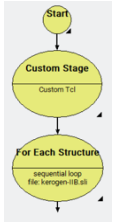
Sorption of CH_4 & CO_2 in kerogen, with swelling

System building (MedeA Molecular Builder, MedeA Amorphous Builder, MedeA LAMMPS) → Solubility calculation & Swelling (MedeA GIBBS & MedeA LAMMPS) → Automation and Analysis

System building

1. Create 10 different initial configurations of a model system containing 10 copies of a kerogen molecule of certain characteristics (maturity, origin…) using the Amorphous Materials Builder at a low density (~0.05 g/ml)
2. Create a structure list containing all 10-20 configurations
3. Use a flowchart to loop over configurations and perform NVT&NPT simulations (including T annealing) to relax at the desired T, P
4. Get the final configurations

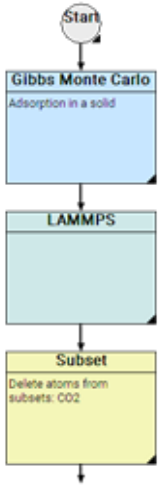


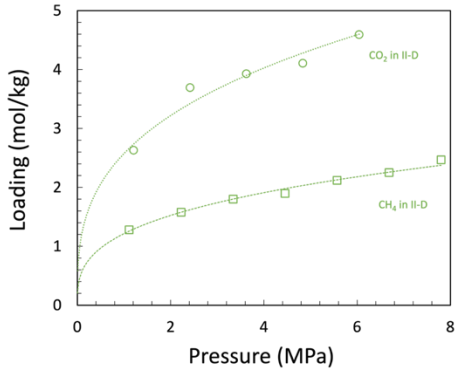


Solubility & Swelling

1. Loop over:
   a. Configurations
   b. Fugacities
2. Inside the fugacity loop:
   a. Sorb gas in the solid (MC)
   b. Relax system including solid and sorbed gas (MD)
   c. Remove the solbed gas
   d. Condinue

Note: Forcefield → pcff+

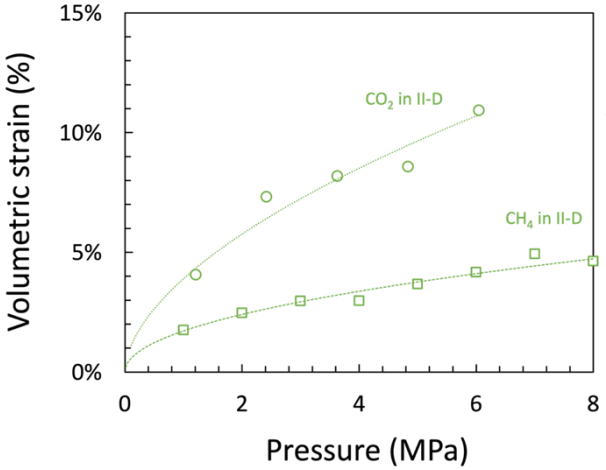




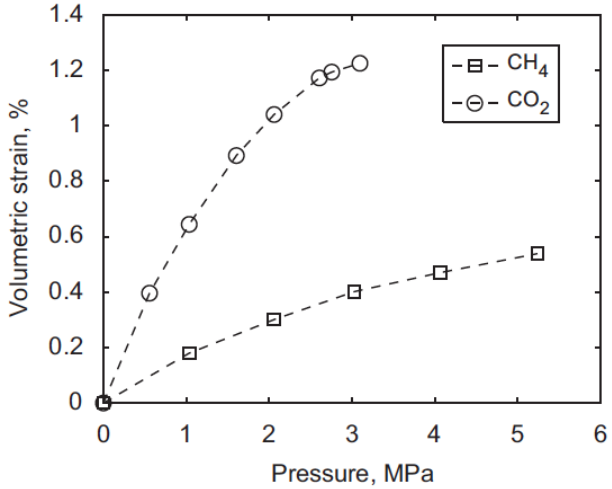
- Simulation results from MC-MD loops.
- Pressure calculated for each value of fugacity of the gas (CH_4 or CO_2) at 300 K, from NPT simulations and Widom test-insertions.
- Each point represents an average from multiple runs in a MC-MD loop.

Volume Strain

- Volume strain: A strain equal to the ratio between the change in volume of an object and its original volume. Also called *bulk strain*.



Simulation results from MC-MD loops. Pressure calculated for each value of fugacity of the gas (CH_4 or CO_2) at 300 K, from NPT simulations and Widom test insertions.

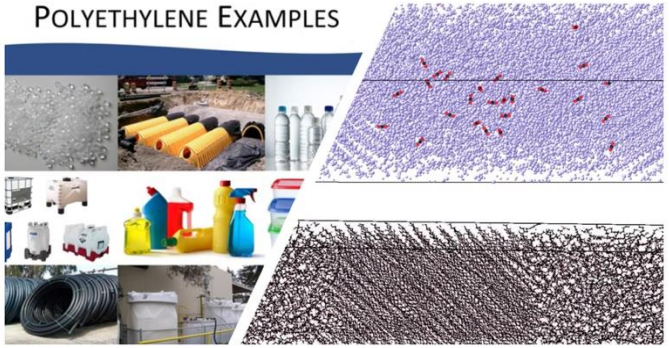


Experimental data on injected coal: volumetric strain versus pore pressure in a CO_2-injected coal and in a CH_4-injected coal (adapted from Vandamme, 2010 where this is reported as adapted from Levine, 1996)

Vandamme et al., Journal of the Mechanics and Physics of Solids 58 (10), p. 1489-1505 (2010)

Levine, Geological Society, London, Special Publications 109 (1), p. 197 (1996)

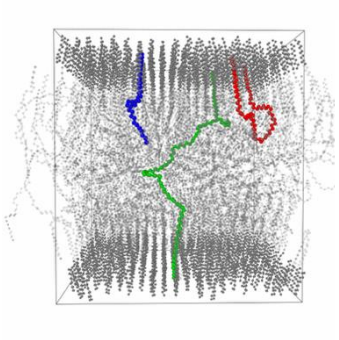
Solubility of CH_4 and CO_2 in semi-crystalline PolyEthylene (PE)

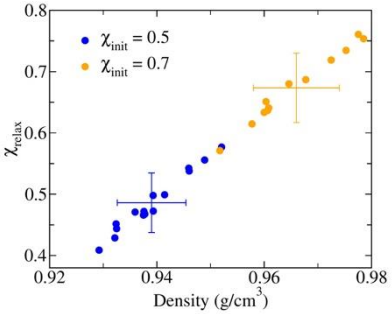


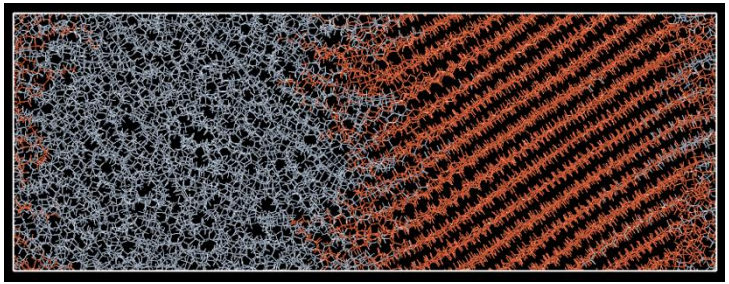
Webinar: B. Belin, *Sorption & Diffusion of Small Gas Molecules in Semicrystalline Models: A Molecular-Scale Investigation*
https://www.materialsdesign.com/webinars

Building realistic HDPE systems

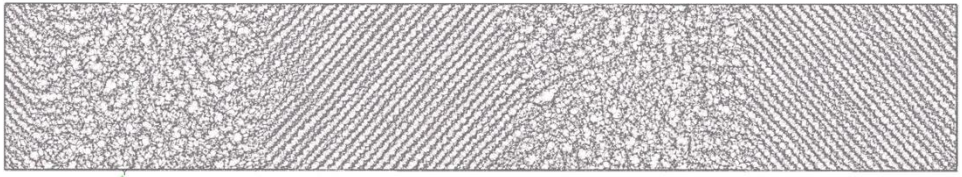
- 2 chains: MW = 140,000 g/mol
- System cross-linking and subsequent relaxation for ~100 ns, at 300 K and 1 atm (MD, NPT)
- Build multiple systems, at different crystallinity degrees







B. Belin et al., J. Phys. Chem. B 126, p. 9673 (2022)

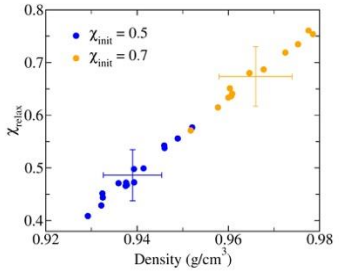


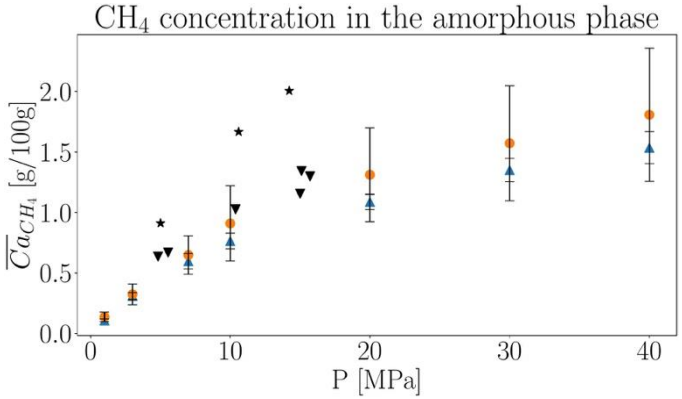
Results averaged over all the structures

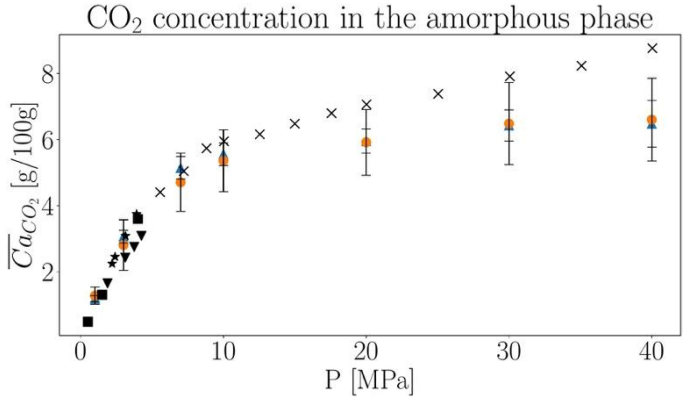
Michaels' Law: $C_a=C/\Phi_a$

Φa: volumetric fraction of the amorphous region

B. Belin, PhD thesis 2023





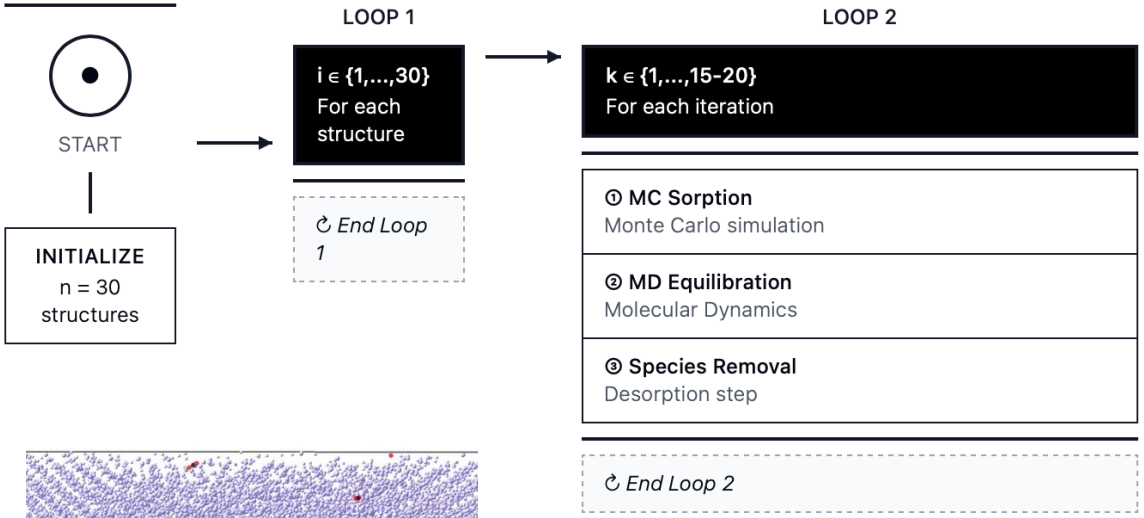


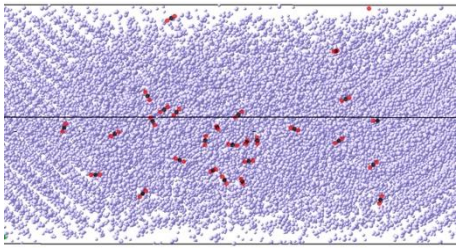
Concentration of CH_4 in the amorphous (▲χ_{init} =50%) and (● χ_{init} =70%) at T=300 K.
Exp. data from: Von Solms et al. (▼,T=305 K) and (★, T=298 K).

Concentration of CO_2 in the amorphous fraction (▲χ_{init} =50%) and (● χ_{init} =70%) at T=300 K.
Exp. data from: a) Von Solms et al. (▼ T=305 K) and (★ T=298 K), b) Flaconnèche et al. (■ T=298 K), and c) Hu (x , T=298 K).

Von Solms, N. et al. Journal of Applied Polymer Science (2004)
Flaconneche, B. et al. Oil & Gas Science and Technology - Revue d'IFP Energies nouvelles (2001)
Hu, T. Permeation of High Pressure CO2 in Semicrystalline Polymers. Phd Thesis. (Imperial College London, 2021)

Simulation Workflow

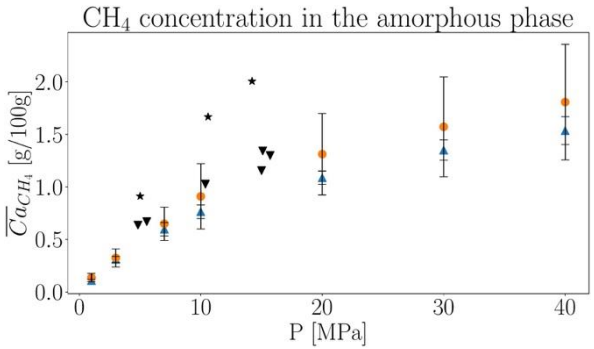




B. Belin, PhD thesis “Relationships between the molecular structure and the mechanical and physico-chemical properties of semicrystalline polymers”, 2023

COMPUTATIONAL SUMMARY

Structures		Iterations		Steps/iteration		Total Operations
30	×	15-20	×	3	=	1,350-1,800



Summary

- The *MedeA*® software environment hosts a variety of versatile tools required for the creation of realistic models of polymer and polymer-containing materials:
  - Bulk polymer
  - Crosslinked resins
  - Interfacial systems and composites
- Integration of highly regarded simulation programs, such as LAMMPS and GIBBS (and others not discussed in this talk, such as VASP, MOPAC, Gaussian, etc.) enables multiple types of property calculation on materials of interest.
- Accurate forcefields, in particular the PCFF+ forcefield developed continuously at Materials Design, and proven property calculation methods are increasingly capable of computing properties with an accuracy comparable with experiment
- Last, but by no means least, the high-throughput oriented design of the environment makes the *MedeA*® platform ideal for computational Polymer Science.

Question and Answer Session

Marianna Yiannourakou

Materials Design

David Rigby

Materials Design

Benoit Minisini

Materials Design

Highlighted *MedeA* Modules

MedeA Environment: The *MedeA*® software package is the leading environment for the atomistic simulation of materials. *MedeA* enables professional, day-to-day deployment of atomic-scale and nano-scale computations for materials engineering, materials optimization and materials discovery. In *MedeA*, world-class simulation engines are integrated with elaborate property prediction modules, experimental databases, structure builders and analysis tools, all in one user-friendly environment.

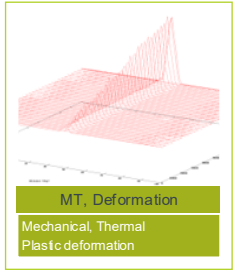
Amorphous Builders: The *MedeA Amorphous Materials Builder* lets you efficiently create condensed phase models based on system chemical or mesoscale composition and target density. It eliminates the need for lengthy mixing and amorphization simulations through realistic sampling of the translational, rotational, and conformational degrees of freedom of component species.

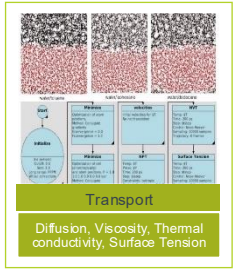
***MedeA* HT:** *MedeA's* HT enables you to generate large and consistent sets of computed data and to create descriptors combining experimental and computed properties to screen, understand, and optimize materials, thus creating the input for machine learning procedures.

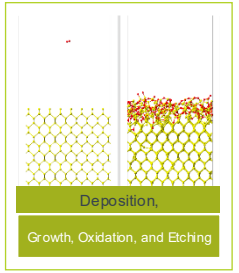
MedeA Diffusion: *MedeA Diffusion* module enhances your diffusion calculations by automatically computing the diffusivity of selected species using atomistic molecular dynamics techniques and facilitates you to observe the diffusive behavior of the different components.

MedeA LAMMPS: *The MedeA LAMMPS module unlocks the power of LAMMPS by providing flexible calculation setup and advanced analysis capabilities, including automatic assignment of forcefield atom types and preparation of coordinate and molecular topology input, identification of required forcefield energy terms along with associated energy expression parameters, and preparation of LAMMPS command input files.*

MedeA GIBBS*: MedeA GIBBS* focuses on the prediction of fluid properties in various equilibrium conditions such as molecular liquids of complex structure, sorption in natural and industrial adsorbents, solubility of small compounds in polymer materials, and ion exchange.







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Related *MedeA* Webinars

Introducing Tailored Polymer Design: Harnessing Molecular Modeling & Data Science:
https://www.materialsdesign.com/webinars/recorded/tailored-polymer-design-harnessing-molecular-modeling-data-science

Molecular Modeling of Kerogen Structure, Thermodynamic and Transport Properties

https://www.materialsdesign.com/webinars/recorded/molecular-modeling-of-kerogen-structure-thermodynamic-and-transport-properties

Use of Polymer Theoretical Concepts in Atomistic Polymer Simulation Software

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De Novo Polymer Design Breakthrough

https://www.materialsdesign.com/webinars/recorded/de-novo-polymer-design-breakthrough

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Related *MedeA* Tutorials

Permeability of O2 in Polystyrene

Absorption of Carbon Dioxide in Kerogen

Adsorption of Methane in Silicalite

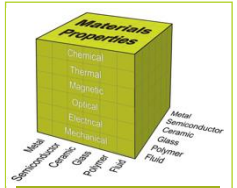
Building Crosslinked Amorphous Polystyrene

Elastic Properties of Polymer and Other Glasses

Building a 2-component Amine-Cured Epoxy Thermoset: DGEBA + JEFFAMINE D-230

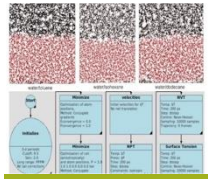
Mechanical Properties of a Thermoset Through Mesoscale Simulations

Building a semicrystalline polyethylene structure



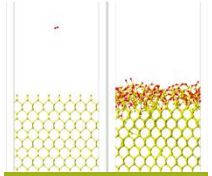
MedeA Environment

Atomistic Modeling and Simulation environment



Transport

Diffusion, Viscosity, Thermal conductivity, Surface Tension



Deposition,

Growth, Oxidation, and Etching

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Question and Answer Session

Marianna Yiannourakou

Materials Design

David Rigby

Materials Design

Benoit Minisini

Materials Design

Questions about Materials Design Webinars

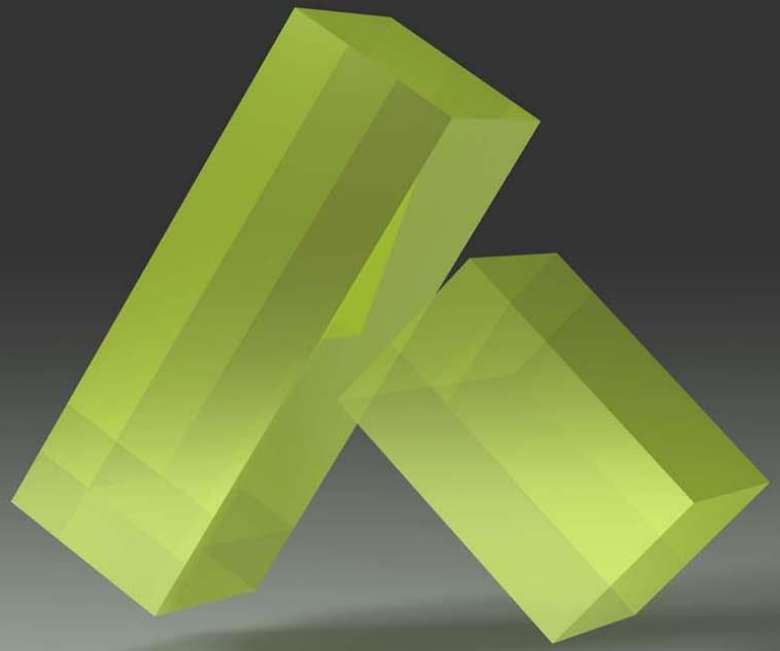
Katherine Hollingsworth

khollingsworth@materialsdesign.com

materials design

info@materialsdesign.com

www.materialsdesign.com



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Innovation by Simulation

Papers Citing *MedeA* and Polymer Applications

2026

- C.A. Martins et al. “Bayesian Optimization for High-Dimensional Coarse-Grained Model Parameterization: A Case Study on Pebax Polymer”, J. Chem. Theory Comput. https://doi.org/10.1021/acs.jctc.5c01500 (**Petronas, Imperial College**)

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- Singh et al. “Molecular Insights into the Protic Organic Ionic Plastic Crystal (POIPC): Effect of Dopants and Vacancies”, ACS Omega https://doi.org/10.1021/acsomega.5c07146 (**Sherbrooke University**)
- Rayhani and Jian “Mechanistic Understanding of the Effects of Graphene Oxide on the Thermal Conductivity of Polymer Fuel Cells”, Proceedings CSME-CFDSC-CSR 2025 (**York University, Canada**)
- Barraud et al. “From soup to structure: Simulating hydrated semi-crystalline proton exchange membranes”, ChemRxiv Sep 22 2025 10.26434/chemrxiv-2025-wmq2v **(IFPEN, Sorbonne University)**
- Liesen et al. “Chain Flexibility and Structure of a Polyimide Copolymer: Revisiting the Freely Rotating Chain Model” Macromolecules https://doi.org/10.1021/acs.macromol.5c00549 **(Lawrence Livermore National Laboratory, US)**
- Robert et al. “Insight Into Supramolecular Interactions of Etherified Alkyl Phenolic Resoles” J. Polymer Science **https://doi.org/10.1002/pol.20241218 (Vikram Sarabhai Space Centre, Cochin University of Science and Technology, India)**
- Hue et al. “Parametric Studies of Polyacrylamide Adsorption on Calcite Using Molecular Dynamics Simulation” Molecules, 2025, 30(2), 285 **https://doi.org/10.3390/molecules30020285 (Imperial College London)**
- W. Müller “The Multiscale Simulation of Graphene Polymer Nanocomposites” PhD report 2025. https://discovery.ucl.ac.uk/id/eprint/10204809/2/Thesis.pdf **(Imperial College London)**
- Laget et al. “Thermo-mechanical properties of sustainable resins through a combined experimental and molecular simulation approach” *Polymer*, 325, 128240 https://doi.org/10.1016/j.polymer.2025.128240 **(Michelin, Université Clermont Auvergne)**
- Suter et al. “Rapid, Accurate and Reproducible Prediction of the Glass Transition Temperature Using Ensemble-Based Molecular Dynamics Simulation” *J. Chem. Theory Comput.* 2025 https://doi.org/10.1021/acs.jctc.4c01364 **(Hexcel Composites, University College London, Université de Rennes)**
- Flottat et al. “Investigating the Influence of the Spacer Length on Anion-Exchange Membrane Properties Using a Reactive Molecular Model” J. Phys. Chem. C 2025, 129, 1, 343–352 https://doi.org/10.1021/acs.jpcc.4c07011 **(Michelin)**
- Khajeh et al. “A materials discovery framework based on conditional generative models applied to the design of polymer electrolytes” *Digital Discovery, 2025, Advance Article* https://doi.org/10.1039/D4DD00293H **(Toyota Research Institute)**

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Papers Citing *MedeA* and Polymer Applications

2024

- Sun et al. “A water-soluble binder in high-performance silicon-based anodes for lithium-ion batteries based on sodium carboxymethyl cellulose and waterborne polyurethane”
  Green Chem., 2024,26, 9874-9887 (**Chinese Academy of Forestry)**
- Larouche et al. “A method for deriving oligomers from sulfamide monomer and their application as electrolytes” Reactive and Functional Polymers, 204, 2024, 106051 https://doi.org/10.1016/j.reactfunctpolym.2024.106051 (**University of Sherbrooke)**
- Sun et al. “A water-soluble binder in high-performance silicon-based anodes for lithium-ion batteries based on sodium carboxymethyl cellulose and waterborne polyurethane”
  Green Chem., 2024,26, 9874-9887 (**Chinese Academy of Forestry)**
- Larouche et al. “A method for deriving oligomers from sulfamide monomer and their application as electrolytes” Reactive and Functional Polymers, 204, 2024, 106051 https://doi.org/10.1016/j.reactfunctpolym.2024.106051 (**University of Sherbrooke)**
- Xu et al. « Transcend the boundaries: Machine learning for designing polymeric membrane materials for gas separation” Chem. Phys. Rev. 5,4, 2024, 041311 **(University of Notre Dame, USA)** https://doi.org/10.1063/5.0205433
- Yang et al. “De novo design of polymer electrolytes using GPT-based and diffusion-based generative models” npj Computational Materials volume 10, Article number: 296 (2024) https://www.nature.com/articles/s41524-024-01470-9 **(Toyota Research Institute)**
- Kroonblawd et al. **“**Developing All-Atom Models of Organic High Explosive Crystal-Polymer Composites**”** *17th International Detonation Symposium Kansas City https://www.osti.gov/servlets/purl/2429371* **(Lawrence Livermore National Laboratory)**
- Singh et al. “A comparative study of polyethylene oxide (PEO) using different coarse-graining methods**”** *J. Chem. Phys.* 160, 224904 (2024) https://doi.org/10.1063/5.0203496 **(University of Sherbrooke, TOTALEnergies)**
- Chen et al. “Dielectric properties of benzocyclobutene-based resin: A molecular dynamics study” J. Phys. Chem. B 2024, 128, 340-349 https://doi.org/10.1021/acs.jpcb.3c06782 **(University of Science and Technology, Mianyang, Sichuan, China)**
- Chen et al. “Effect of Repeat Unit’s Composition Ratio on the Properties of a Random Copolymer: A Molecular Dynamics Simulation Study” *J. Macromolecules Sci, B*, https://doi.org/10.1080/00222348.2024.2325789 **(University of Science and Technology, Mianyang, Sichuan, China)**
- Bicerano et al. “Polymer expert – A software tool for de novo polymer design”, *Computational Materials Science, 235, 2024, 112810* https://doi.org/10.1016/j.commatsci.2024.112810 **(MD)**
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Papers Citing *MedeA* and Polymer Applications

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- Lei et al. “A Self-Improvable Polymer Discovery Framework Based on Conditional Generative Model” https://doi.org/10.48550/arXiv.2312.04013 **(Toyota Research Institute)**
- Yang and al. “De novo Design of Polymer Electrolytes with High Conductivity using GPT-based and Diffusion-based Generative Models” https://doi.org/10.48550/arXiv.2312.06470 **(Toyota Research Institute)**
- Khajeh et al. “Early prediction of ion transport properties in solid polymer electrolytes using machine learning and system behavior-based descriptors of molecular dynamics simulations”, https://doi.org/10.1021/acs.macromol.3c00416(**Toyota Research Institute**)
- Hue et al.” Molecular Dynamics Simulation of Polyacrylamide Adsorption on Calcite” https://doi.org/10.3390/molecules28176367 **(Petronas)**
- Flottat, B. Latour, F. Goujon, P. Hauret, P. Malfreyt “Investigating percolation and clustering effects on aquivion and nafion membranes at the molecular scale” Intern. J. Hydro. Ener. 2023 https://doi.org/10.1016/j.ijhydene.2023.05.086 **(Michelin, Institut de Chimie de Clermont-Ferrand)**
- Shamsieva et al. “Amorphous Cis-1,4-Polybutadiene P-V-T properties from atomistic simulatio” 10.21203/rs.3.rs-2815978/v1 preprint **(MD, Kazan University)**
- Carrola et al. “Fundamentals of Crystalline Evolution and Properties of Carbon Nanotube-Reinforced Polyether Ether Ketone Nanocomposites in Fused Filament Fabrication” ACS Appl. Mater. Interfaces 2023 https://doi.org/10.1021/acsami.3c01307 **(Texas A&M University)**
- Minisini; A Soldera “Volumetric and Energetic Properties of Polystyrene and Polyethylene Oxide Affected by Thermal Cycling” Macromolecular Theory and Simulations https://doi.org/10.1002/mats.202300008 **(MD, Sherbrooke University)**
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High-Throughput Molecular Simulations for Gas Sorption in Polymers

Automated Workflows for Industrial Materials Design