



Molecular simulation as an ideation engine for materials R&D

Hypotheses become quantifiable design rules for molecules, polymers, bulk materials and interfaces

Automation built around accurate energy calculations, aimed at the property that matters

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Materials teams need a faster path to performance targets from chemistry

Start with design space

Define ground-truth availability, determine what aspects can be varied, connect the desired performance property to computable phenomena

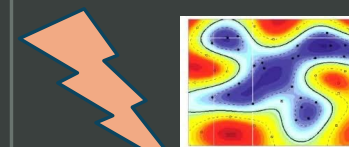
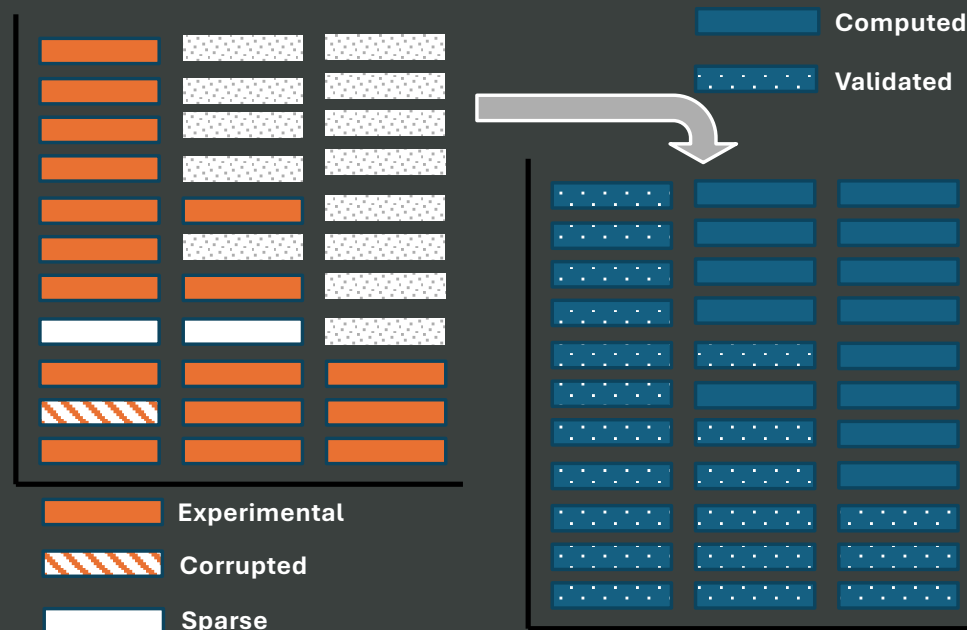
Model the governing physics

Build atomistic representations of molecules, polymers, surfaces and morphology.

Return design rules

Quantify which chemical features control performance and rank the next experiments to test.

Augmenting Laboratory Data

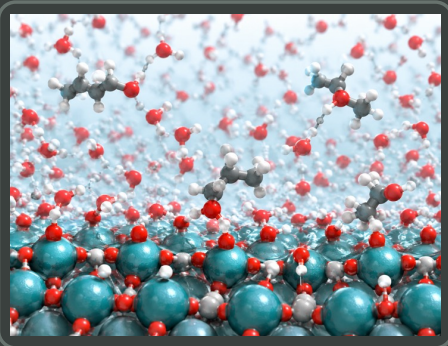


Performance (Property)



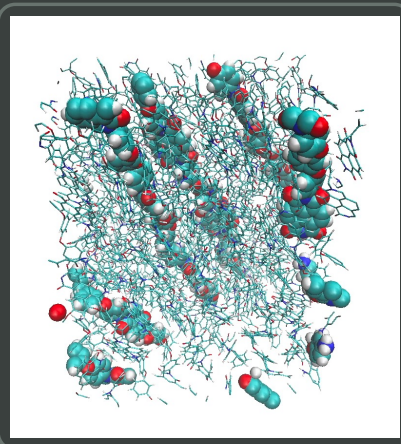
Chemistry (Material)

One workflow supports four materials domains



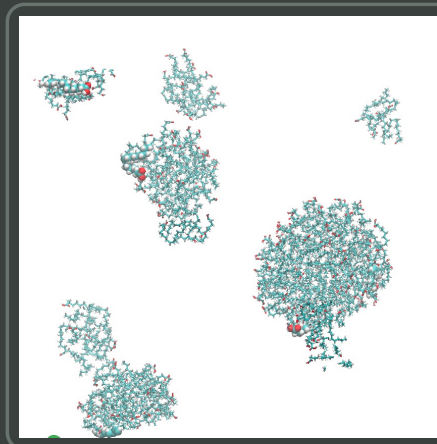
Interfaces and adhesion

Which functional groups anchor to a surface, and under what conditions?



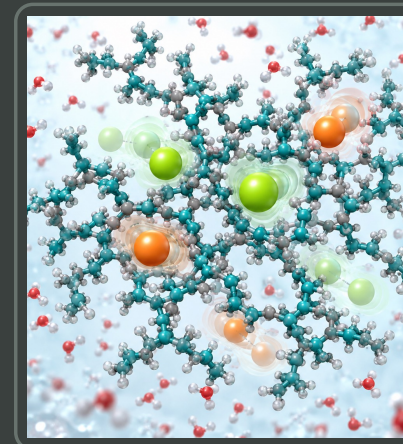
Bulk polymer properties

How do chemistry and morphology affect transition temperatures and phase behavior?



Self-assembly and supramolecular physics

What structures emerge, and which molecular changes shift the outcome?



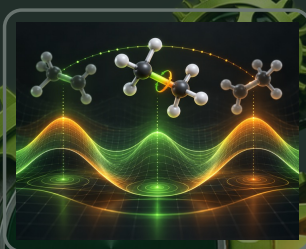
Adsorption and Incorporation

Which interaction motifs drive affinity and selectivity in complex media?

One workflow connects molecular mechanisms to material performance

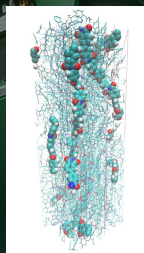
From electronic structure to material behavior

Quantum chemistry



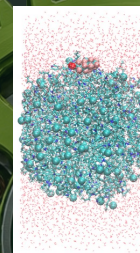
Charges, conformers and interaction parameters grounded in electronic structure

Molecular models



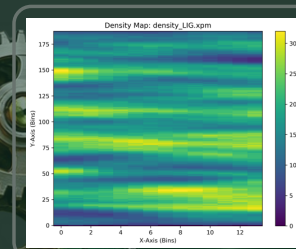
Robust models of materials systems configured to capture essential design criteria

Simulation



Molecular dynamics, free energy and statistical analysis to ideate and optimize materials performance

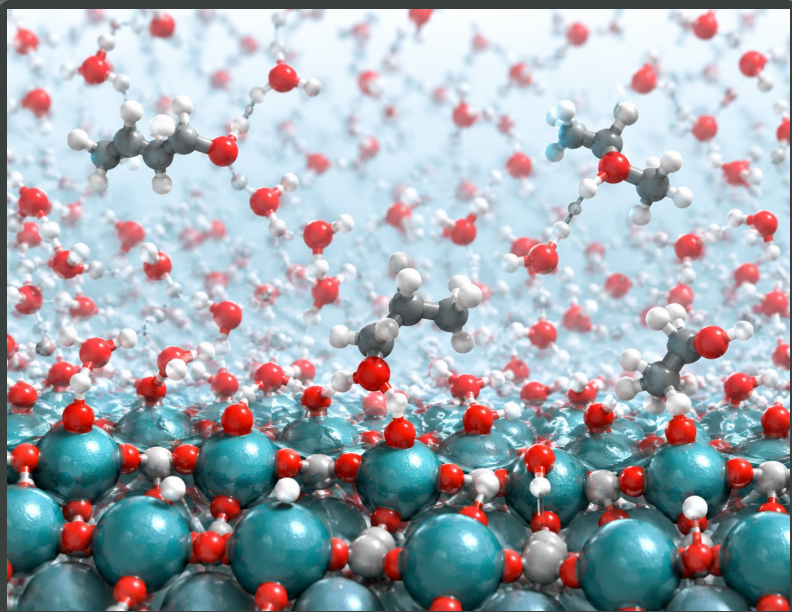
Design insight



Mechanisms, property predictions tell us what governs performance and how to decide which direction to move in

From hypothesis to quantitative, self-consistent data for design

Case study: atomistic models explain surface affinity and adhesion



Industrial question

Which molecular features improve adhesion to a chemically complex surface?

Model

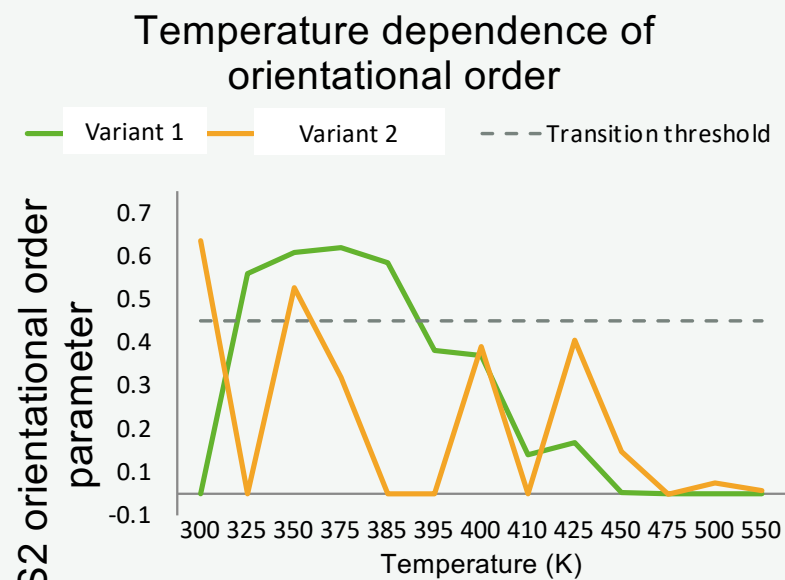
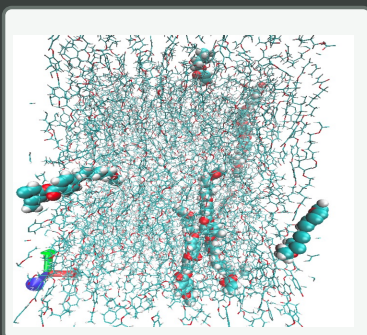
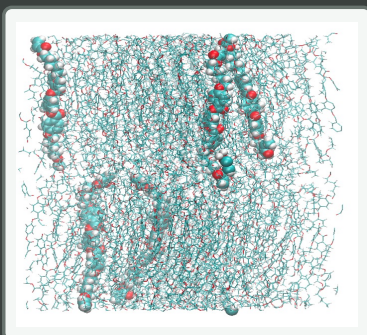
Quantum-informed parameters and explicit molecular dynamics resolve multiple binding modes and solvent effects over time detailing the dynamics and statistics of adhesion.

Decision

The simulation identifies the dominant interaction motif and shows where chemical modification can improve retention.

From an attractive hypothesis to a quantified binding mechanism

Orientational order reveals temperature-dependent phase stability



Challenge

Determine when candidate lyotropic structures lose orientational order as temperature increases.

Model

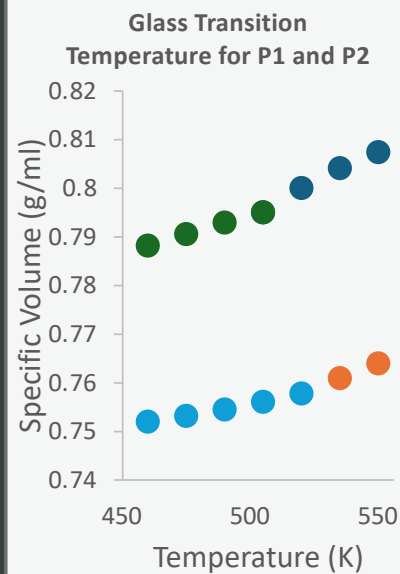
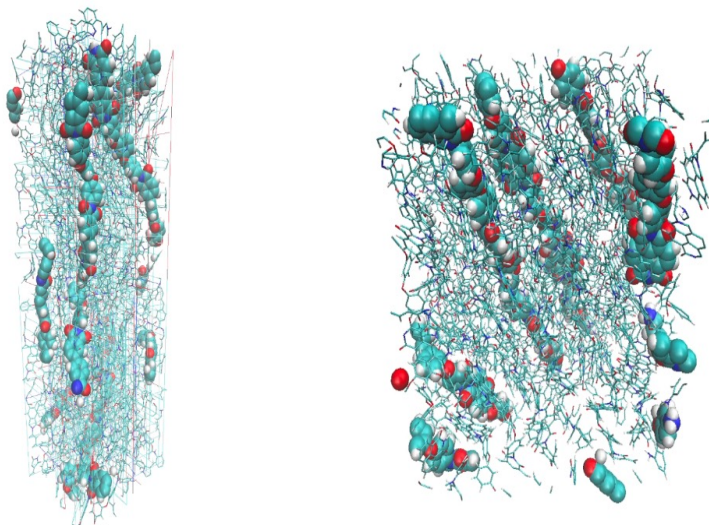
Temperature-resolved molecular dynamics tracks the S2 order parameter across native and designed materials.

Decision

Compare transition windows before synthesis and prioritize structures that retain order under operating conditions.

Simulation converts molecular trajectories into a quantitative phase-transition window

Polymer structure predicts glass-transition behavior



Challenge

Predict how two related copolymer architectures change mobility and packing across temperature.

Model

Simulated annealing and density analysis reveal the glass-transition regime for each atomistic model.

Decision

Use the predicted transition range to rank formulations before experimental thermal analysis.

One atomistic workflow links polymer structure to bulk-transition behavior

One resin model expanded into 110 independent PFAS-bulk incorporation simulations

We parameterized a novel ion-exchange resin once, then reused the validated build and simulation pipeline across a structured design matrix.

110 INDEPENDENT SIMULATIONS

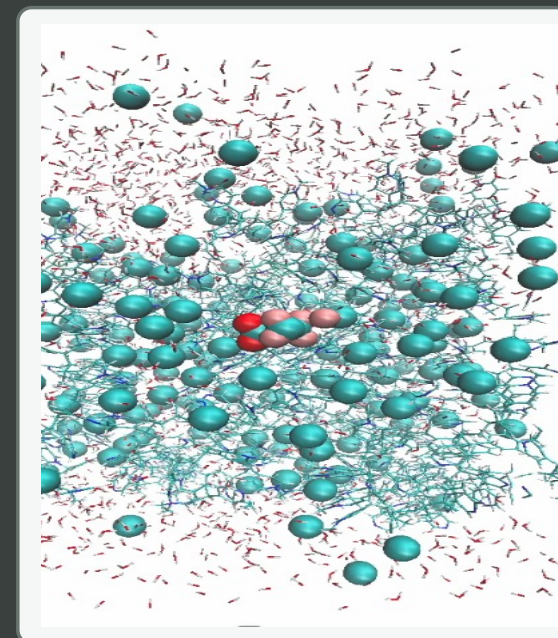
The design matrix varied

PFAS identity

**Resin
quaternization**

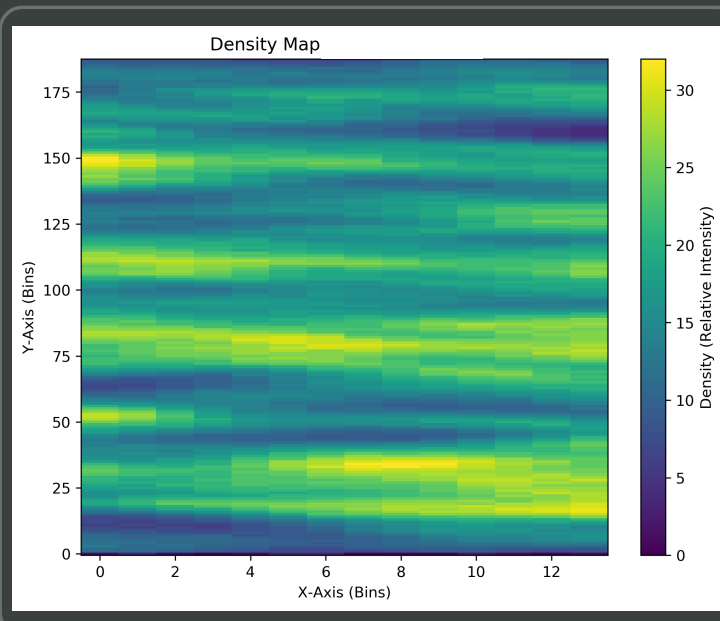
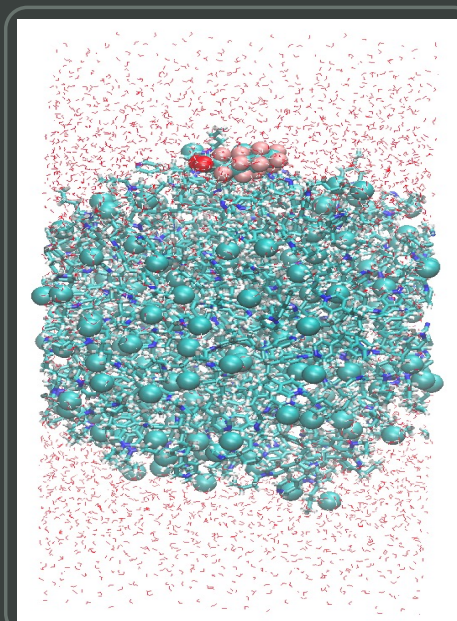
**Alkyl chain
length**

One model-building effort became a comparative dataset for material design.



A validated resin model becomes a reusable design platform to understand and control material performance

Charge, hydration and morphology control PFAS capture



Model the complete material

Cross-link density, ion-exchange loading and water distribution determine whether PFAS can reach favorable regions.

Resolve chain-length selectivity

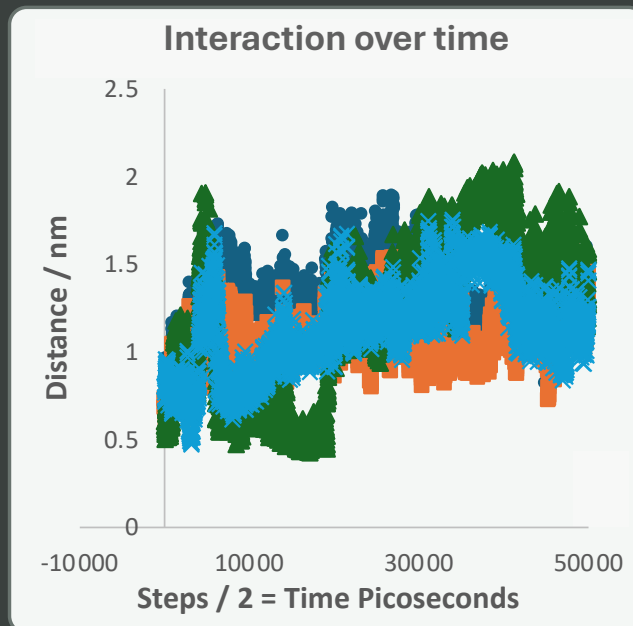
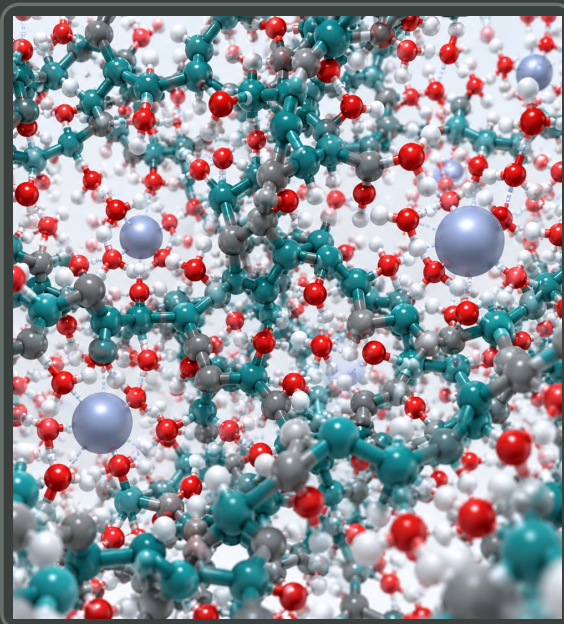
Explicit PFAS structures reveal how electrostatics and hydrophobic association contribute differently across the series.

Define a design window

The result identifies which matrix properties should move together to improve capacity without losing accessibility.

A complete material model defines the design window for PFAS capture

PFAS simulations reveal actionable design rules



Interaction balance

Electrostatic attraction contributes only when charged sites remain accessible through the hydrated matrix.

Hydration constraint

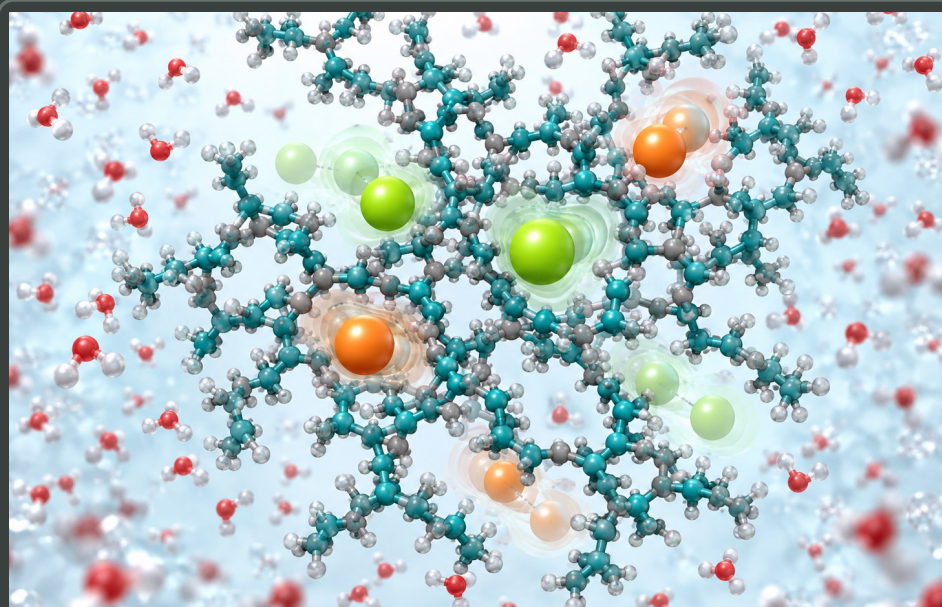
Excess water uptake screens local interactions and reduces effective contact with the binding environment.

Design implication

Tune functionalization to preserve access without over-wetting. The preferred balance shifts with guest size.

Mechanistic insight narrows the experimental search space

Dendrimer models expose realistic PFAS binding microstates



Enumerate realistic states

Conformations, protonation states and PFAS chain lengths generate a distribution of binding microstates.

Thermodynamic Integration

Free-energy calculations separate hydration penalties from favorable host-guest interactions and give a single usable value for dendrimer design ranking.

Guide synthesis

Comparing the microstates identifies where branching, charge placement or local hydrophobicity can improve selectivity.

Microstate populations reveal which molecular changes can improve PFAS selectivity

Paid pilots create repeatable prediction workflows

1 Scope

Define the decision, target property and experimental evidence available.

2 Build

Construct and parameterize the material model around the actual operating conditions.

3 Validate

Compare the simulation with known behavior and document the limits of prediction.

4 Apply

Use the validated workflow to rank new molecules, formulations or process conditions.

The client owns the decision framework; ChemAlive carries the model development and computation

Bring us the materials challenge that is slowing your program

We will define the simulation that will uncover the blocking issue and help optimize your material performance.

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