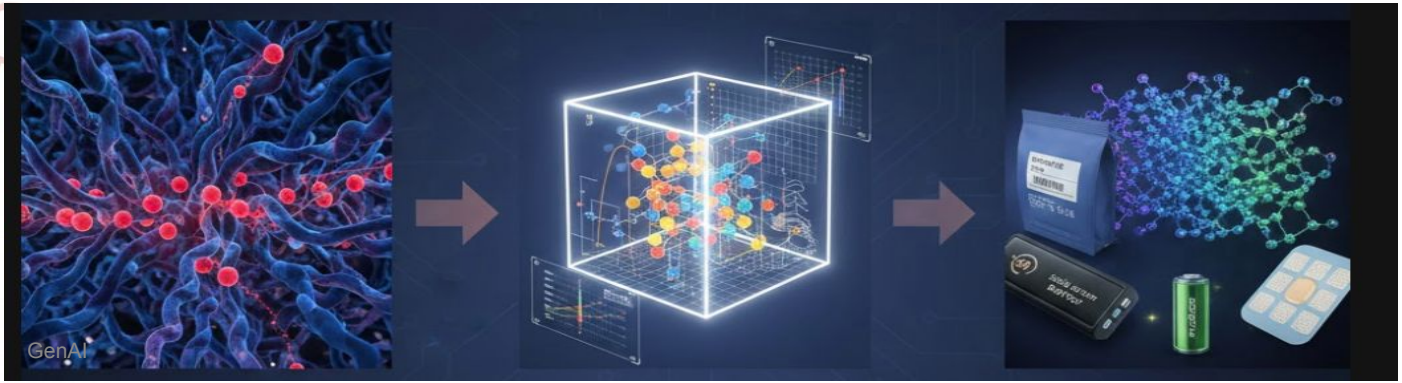
Predictive Modeling for Polymer Diffusion

Connecting Microstructure to Macroscopic Barrier Performance



The Challenge:

Unpredictable molecular migration leads to microstructural failure that traditional testing cannot see or isolate.

The Solution:

Uses Molecular Dynamics to track migration pathways and predict the Diffusion Coefficient (D) before physical synthesis.

J-OCTA

Integrated system for multiscale Modeling and Simulation

Strategic Impact:

- Accelerated R&D
- Cost Reduction
- Industry Ready

The Challenge

The performance and lifespan of polymers are limited. This limitation arises because **small molecules and ions** (like oxygen, water, or drug compounds) inevitably **migrate through the material by diffusion**.

Traditional Testing (Macroscopic)

- **Slow & Costly:** Slow and expensive (e.g., gravimetric analysis)
- **Core Limitation:** Cannot isolate the microstructural origin of poor performance.



Application Failure Risks

- **Safety Hazards: Critical risk in** food packaging and pharmaceuticals
- **Costly Regulatory Failures**



The Solution

Connecting Microstructure to Macroscopic D

Atomistic simulations provide direct insight into how the microstructure (e.g., free volume, chain dynamics) **controls the movement of diffusing molecule**.

By accurately modeling the polymer structure and the energy barriers to movement, you can virtually predict the Diffusion Coefficient for new materials before synthesis and testing.



The simulation provides physics-based parameters like:

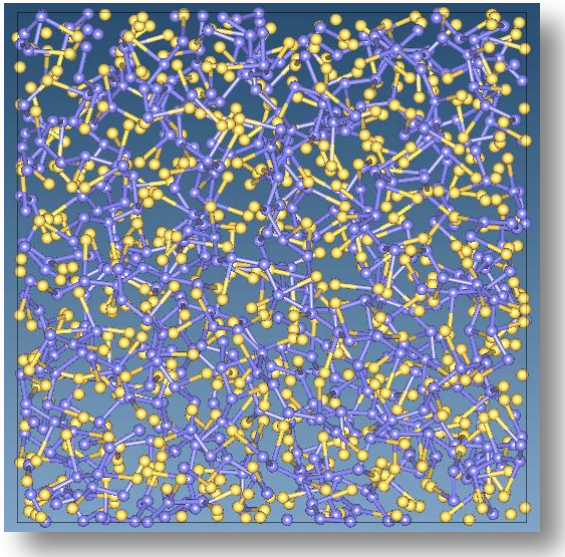
- **Diffusion Coefficient** (D): This is the ultimate macroscopic performance metric.
- **Migration Pathway**: Describe the path a small molecule takes through the polymer matrix.

The Solution

J-OCTA is **multi-scale simulation software** for predicting properties of high-performance materials f**rom the atomistic to the micrometer scale**.

J-OCTA addresses the diffusion challenge by creating a **realistic amorphous polymer structure** and using advanced methods like **Molecular Dynamics** to calculate key physical data governing molecular migration.

The software determines the **Diffusion Coefficient** by accurately tracking individual molecule movement, providing direct insight into **how the microstructure controls macroscopic performance**



J-OCTA
Integrated system for multiscale Modeling and Simulation

GET A QUOTE & SCHEDULE A DEMO

Impact



Accelerated Development

Rapidly screen new polymer compositions or additives to predict performance (e.g., barrier properties, ion conductivity).

Reduced Testing

Cuts reliance on costly and lengthy experiments for material qualification by providing validated, physics-based data.

Optimized Applications

Energy Storage:
Optimize ionic conductivity for solid-state batteries.

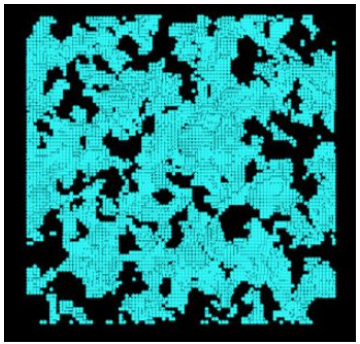
Pharmaceuticals:
Determine the rate of drug diffusion through delivery matrices.

Filtration:
Optimize selective transport for water treatment.

Related Case Studies: Gas Solubility

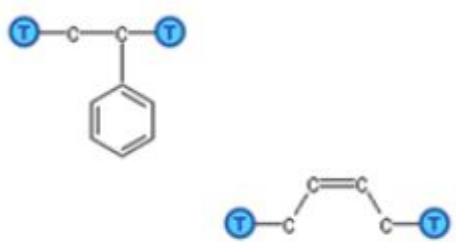
The following case studies cover gas solubility in polymer matrices. Solubility, together with molecular diffusion, governs gas transport and ultimately controls permeability.

“Gas Solubility Coefficient and Free Volume”



VIEW CASE STUDY

“Calculation of Solubility Coefficient”



VIEW CASE STUDY

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Next Steps: Start Your Atomistic Simulation

Test The Technology

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Solve the Challenge

Schedule a Free Strategic Consultation: Discuss your material challenge with our scientific team

Contact us: team@simuneatomistics.com



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