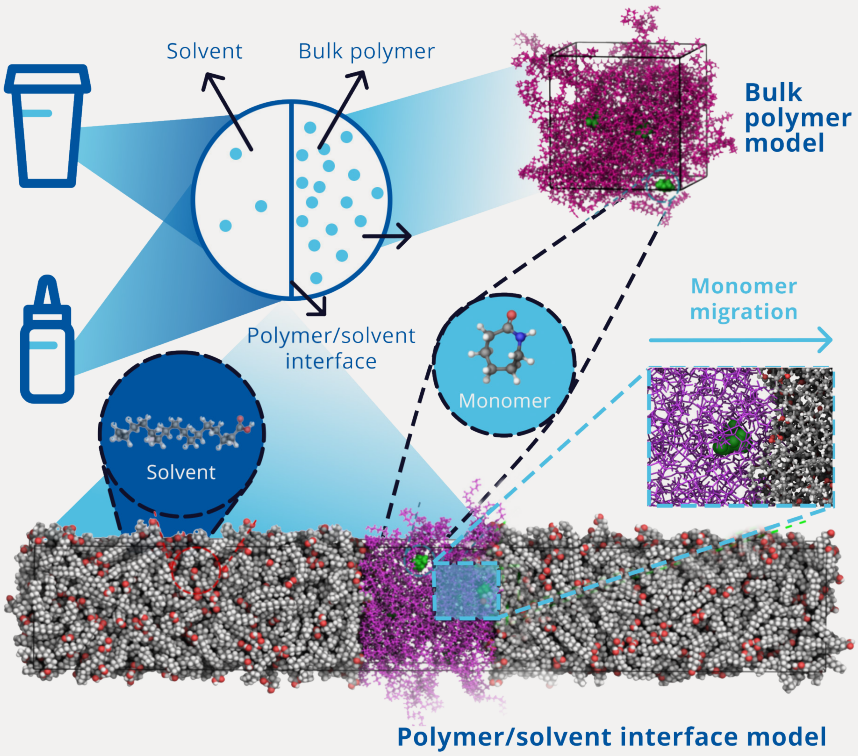
CASE STUDY

Designing better packaging materials with a reduced risk of contamination and longer shelf-life using molecular simulations

Molecular dynamics simulation of plastic contaminant migration in packaging materials and potential leaching into model food fluids

Executive Summary

- Built and validated a molecular model that can predict bulk and interfacial penetrant diffusion, as well as enable an understanding of the underlying mechanisms governing these processes
- Established a modeling procedure to successfully carry out the challenging simulations of migration processes within and from polymer phases
- Gained valuable insights to complement and rationalize labor- and time-intensive penetrant migration experiments for product developers, regulatory agencies, and manufacturers



Examples of bulk and interfacial structures employed in the molecular modeling of penetrant diffusion in polymeric systems.

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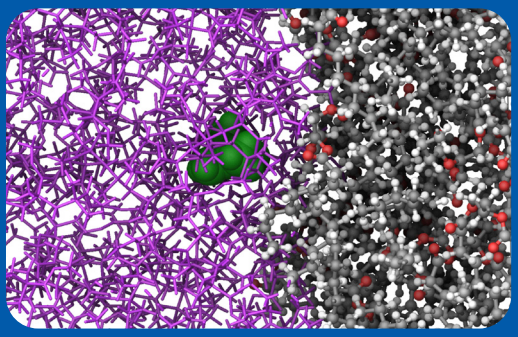
Approach

In Mileo et al., Schrödinger scientists employed molecular dynamics (MD) simulation using the Schrödinger Materials Science Suite, Desmond MD engine and the OPLS4 force field. The goal of this work was to analyze the transport of monomers in three commercially important, recyclable polymers: polyamide-6 (PA 6), polycarbonate (PC), and poly(methyl-methacrylate) (PMMA). To achieve this, scientists performed the following steps:

1. Validated bulk polymeric models with respect to properties derived from experimental work
2. Verified the predictability of the modeling strategy in reproducing the experimental monomer migration tendencies by employing different solvents to simulate foodstuff
3. Predicted the monomer migration mechanism in two typical components employed in the food industry (palmitic acid and capric triglyceride)

Conclusion

This work demonstrates how molecular-scale insights can aid the design of safe and functional polymer/formulation interfaces in industry-relevant consumer goods. The methods presented can also be leveraged to understand the risk of contaminants leaching into food or other consumer products, alongside understanding how the product itself can impact the rate of contamination at a barrier interface.



Snapshot obtained from MD simulation displaying the imminent migration of a monomer (methyl methacrylate, in green) from its polymer matrix (polymethyl methacrylate, in purple) towards a palmitic acid formulation.

Publication

1. Mileo PG, et al. Nanoscale Simulation of Plastic Contaminants Migration in Packaging Materials and Potential Leaching into Model Food Fluids, *Langmuir* 2024, 40, 24, 12475–12487

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