CASE STUDY

Prediction of Moisture Adsorption and Effects on Amorphous Amylose Starch

Molecular Dynamics simulations accelerate optimization of product quality and processing for food and beverage, packaging, and pharmaceutical applications.

Executive Summary

- **Accurately predicted key physical properties** such as glass transition temperature (T_g) for both wet and dry amorphous amylose polymers
- **Effectively modeled water uptake and transport** by investigating the effect of moisture content on T_g and water diffusion in starch polymers
- **OPLS3e force field provided high accuracy** for amorphous starch models
- **Further studies proposed** on in-depth water-amylose interactions and the effects of ingredients on complex starch formulation

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Challenges

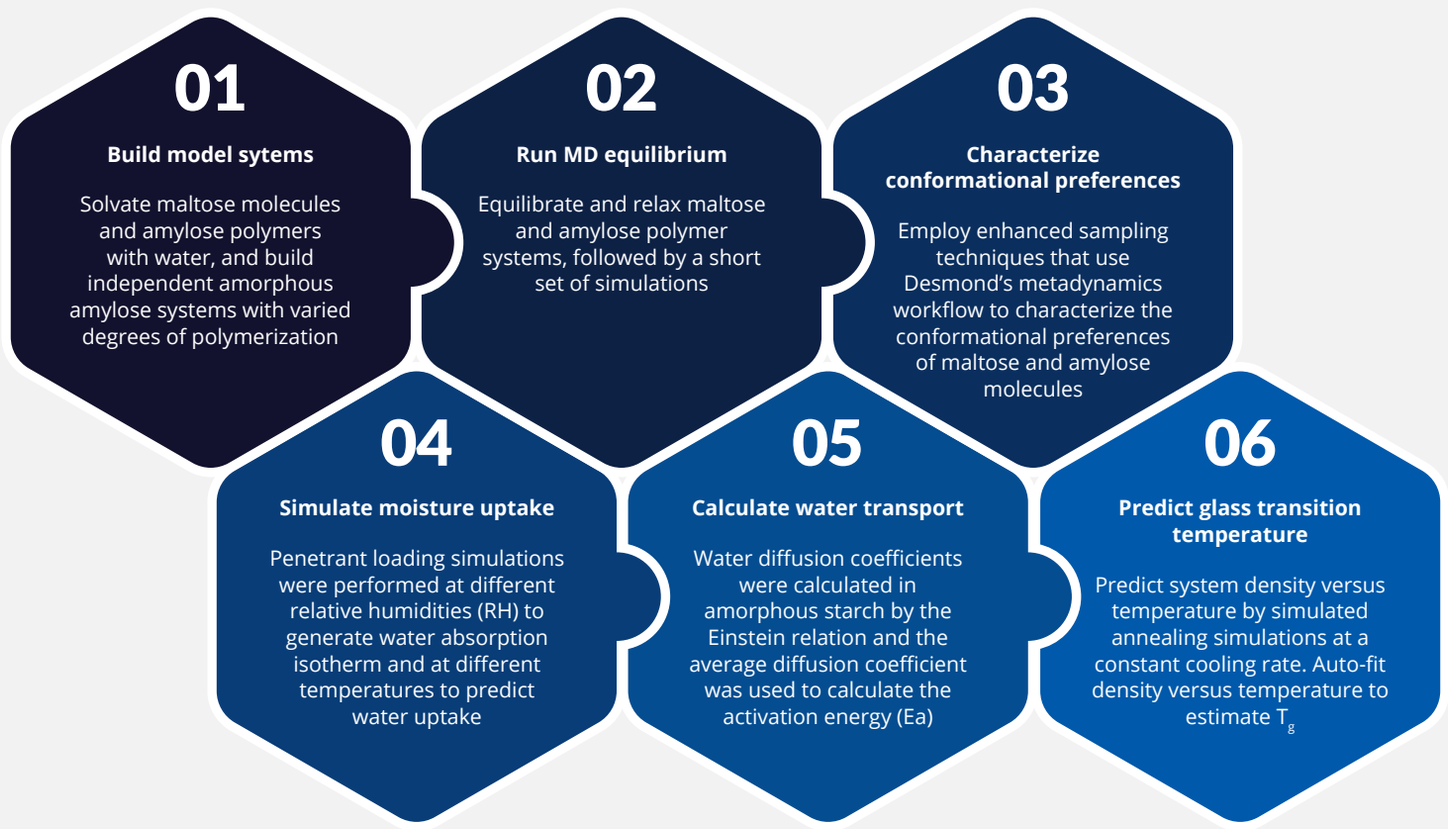
As amorphous starch is highly attractive for applications in thermoplastics and food encapsulation, understanding its functionality is a high priority for R&D scientists in several industries. Key to starch functionality is the interaction between water and starch granules. Numerous studies have focused on understanding the microstructure and the underlying nanostructure of starch, however a thorough understanding of the molecular structures of native and amorphous granules is challenging to characterize experimentally. This results in:

- Lack of high resolution, atomic level structural characterizations
- Lack of morphological or thermophysical properties of amorphous starch
- Lack of dynamic properties of amorphous starch in solvent

Approach

Scientists at Schrödinger aimed to solve these challenges by using molecular simulation techniques, specifically molecular dynamics (MD) simulations.[1] All models and simulations were performed using the Schrödinger Materials Science Suite. These methods predicted water uptake at a given temperature and relative humidity condition and also allowed for tracking of water transport in the starch polymer matrix.

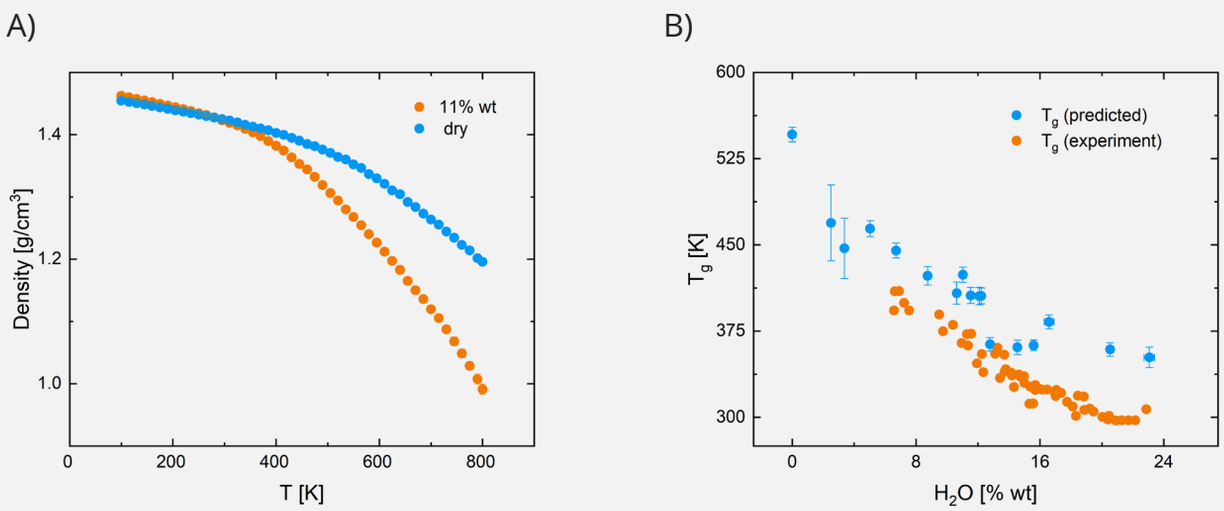
Seamless Workflow with Schrödinger's Intuitive Modeling Platform for Materials Science



Results

MD simulations have greatly improved our understanding of amylose molecules in solution and bulk phase and have led to rapid prediction of key physical properties such as T_g.

- The results illustrate the plasticization effect of moisture content on amorphous starch. Predicted glass transition temperature (T_g) depression as a function of moisture content is in line with experimental trends and allows prediction of the previously inaccessible dry T_g of amorphous starch.
- Using combined grand canonical Monte Carlo (GCMC)/MD simulations, a moisture sorption isotherm curve is predicted along with temperature dependence. Concentration-dependent activation energies for water transport agree quantitatively with previous experiments.
- The modern OPLS3e force field and well-tempered metadynamics provided highly accurate prediction of dynamical properties and conformations for amorphous starch polymers in addition to solution behavior.



Plasticization effects of water on amorphous DP31 amylose. A) Density versus temperature plots of dry and 11 % moisture content DP31 using a 0.67 ns/K cooling rate. B) T_g as a function of moisture content. Blue data points represent the average of five independent systems. Orange data points are experimental values reported in (Ai & Jane, 2018).*

What's Next?

- Further studies can explore in-depth water-amylose interactions and the effects of other commonly used ingredients in starch formulations, for example emulsifiers, which are known to bind to amylose molecules.
- Future work can be performed to understand the morphology of complex amorphous and/or semi-crystalline starch formulations and how morphology affects transport and thermomechanical properties.

References

1. Jeffrey M.Sanders, Mayank Misra, Thomas J.L.Mustard, David J.Giesen, Teng Zhang, John Shelley, Mathew D.Halls, "Characterizing moisture uptake and plasticization effects of water on amorphous amylose starch models using molecular dynamics methods", *Carbohydrate Polymers*, 252, 2021, 117161.

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