

Polymer films composed of chitosan/chitin are promising materials for sustainable polymer packaging. In the case of food packaging, the key requirement is impermeability to oxygen ( $O_2$ ). Under dry conditions, chitosan films are impermeable to oxygen, however when hydrated they become increasingly more permeable. In this study, molecular models were created of 67% chitosan (poly(N-glucosamine)) and 33% chitin (poly(N-acetylglucosamine)) to reproduce the composition of typical experimental films. The films were hydrated at low and high relative humidities (RH) of 0.15 and 0.95 in order to simulate the transport of oxygen under varying conditions of humidity. The systems are simulated using classical molecular dynamics (MD), in which the trajectories of each atom are followed through time. MD simulations provide insight into the configurational changes of the polymer as a result of the absorption of water; these configurational changes impact  $O_2$  transport through the film. The objective is to develop the molecular-level insight into the mechanism by which the presence of high humidity enhances oxygen transport. This understanding will be communicated to a polymer film synthesizer in order to design a processing step which modifies the nanostructure of the polymer film, eliminating or reducing its oxygen permeability under all humidity conditions.