Molecular-level simulations of permeation in polymer films and fibres

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The permeability of small penetrant molecules in polymer materials is important for many applications, *e.g.*, fuel cells, gas separation and packaging. Polyethylene (PE) and polyvinylalcohol (PVA) are, for example, widely used for packaging materials and their barrier properties towards penetrants such as oxygen and water is a factor that determines the shelf-life of the packaged product. It is therefore important to identify the polymer properties that affect the permeation of penetrants. This will assist in developing new polymers that have desired barrier properties.

Molecular-level computer simulations have been performed to calculate solubility, S, and diffusion, D, coefficients of water and oxygen in PE and PVA, and to obtain a molecular-level understanding of the diffusion mechanism. The permeation coefficient, P, was calculated from the product of S and D. The figure below shows that the simulated S for water in PE yields the correct trend of increasing S with increasing temperature, although the simulated values are lower than the experimental data. The calculated diffusion coefficients are in good agreement with experimental data. The correct trend observed for the simulated S and D is reflected in the correct trend seen for P. Diffusion occurs mainly by large amplitude, infrequent jumps of the molecules through the polymer matrix.

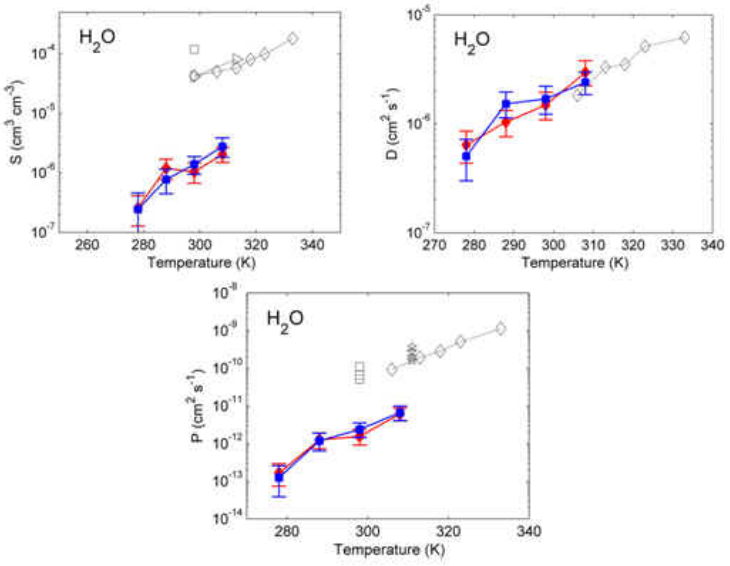

Figure: Solubility (top left), diffusion (top right) and permeability (bottom) coefficients of water in PE. The simulated results are shown with error bars (squares are when atomic charges are included in the force field) and experimental results are shown in grey.

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