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Molecular Dynamics Simulations of Gas Transport in Polymer Films DAVID WHITLEY, SIMON BUTLER, DAVID ADOLF, School of Physics and Astronomy, University of Leeds, UK — Parallel molecular dynamics simulations have been carried out to determine the permeability of O_2 and N_2 through polyethylene terephthalate, polypropylene and cis(1-4) polybutadiene. The permeability of both mixed and unmixed gas penetrants is studied within films of these well known gas barrier polymers. Results are obtained either through the solubility and diffusion (i.e. $P = D * S$) or via the permeability directly. Encouraging results are obtained. Additional analysis focuses on "unmixed/mixed gas" intracomparisons of the simulated permeability data in addition to corresponding penetrant and host polymer local dynamics.

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