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Gas Diffusion in Polyethylene Terepthalate By Molecular Dynamics[1] SIMON BUTLER, DAVID ADOLF, School of Physics & Astronomy, University of Leeds, Leeds, LS2 9JT, UK — Molecular dynamics simulations of the diffusion of small penetrants through PET have been performed utilising the anisotropic united atom model [1] and a virtual liquid technique. [2] The accuracy and reliability of these two approaches has been assessed in terms of the improvement in equation of state behaviour and of diffusion co-efficients and solubilities. The effect of the diffusion of nitrogen, carbon dioxide, and oxygen on the local dynamics of PET have been investigated as a result. Attention has been focused on the dual mode effect [3] observed during mixed gas diffusion.

[1] *Molecular dynamics calculation of the equation of state of alkanes*, J. Chem. Phys. *93*, 6 (1990)
[2] Kikuchi, Kuwajima, Fukada, *Novel method to estimate the solubility of small molecules in cis-polyisoprene by molecular dynamics simulations*, J. Chem. Phys, *115*, 13 (2001)
[3] Lewis, Duckett, Ward, Fairclough, Ryan, *The barrier properties of polyethylene terephthalate to mixtures of oxygen, carbon dioxide and nitrogen*, Polymer, *1631*, 44 (2003)

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Simon Butler
School of Physics & Astronomy, University of Leeds, Leeds, LS2 9JT, UK

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