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A molecular study of gas solubility in nitrile rubber MUSAB KHAWAJA, Imperial College London, Department of Physics, London SW7 2AZ, UK, ARASH MOSTOFI, Imperial College London, Departments of Materials and Physics, London SW7 2AZ and the Thomas Young Centre for Theory and Simulation of Materials, UK, ADRIAN SUTTON, Imperial College London, Department of Physics, London SW7 2AZ, UK — One of the most important uses of elastomers in the oil industry is for seals to encase and protect sensitive monitoring equipment from contamination by gases and liquids at the high pressures and temperatures in the well. Failure of such seals sometimes occurs on decompression when they are returned to the surface. The conditions in the well lead to gases being absorbed by Nitrile rubber (NBR) seals. NBR exhibits a strong permselectivity towards CO2 compared to other gases; something attributed experimentally to the enhanced solubility of CO2. In this study an explanation is sought at the molecular level for this phenomenon. A series of molecular mechanics calculations are performed to compute solubilities of different gases in NBR. The effect of acrylonitrile content on their solubilities is studied for the first time by simulation, and we discuss the important issue of convergence with respect to the sampling of different elastomer configurations. It is observed that the presence of cyano groups has a marked impact on the solubility of CO2 and an explanation is offered.

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