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Predicting the solubility of gases in Nitrile Butadiene Rubber in extreme conditions using molecular simulation MUSAB KHAWAJA, NICOLA MOLINARI, ADRIAN SUTTON, Imperial College London, Department of Physics and the Thomas Young Centre for Theory and Simulation of Materials, UK, ARASH MOSTOFI, Imperial College London, Departments of Materials and Physics and the Thomas Young Centre for Theory and Simulation of Materials, UK
— In the oil and gas industry, elastomer seals play an important role in protecting sensitive monitoring equipment from contamination by gases - a problem that is exacerbated by the high pressures and temperatures found down-hole. The ability to predict and prevent such permeative failure has proved elusive to-date. Nitrile butadiene rubber (NBR) is a common choice of elastomer for seals due to its resistance to heat and fuels. In the conditions found in the well it readily absorbs small molecular weight gases. How this behaviour changes quantitatively for different gases as a function of temperature and pressure is not well-understood. In this work a series of fully atomistic simulations are performed to understand the effect of extreme conditions on gas solubility in NBR. Widom particle insertion is used to compute solubilities. The importance of sampling and allowing structural relaxation upon compression are highlighted, and qualitatively reasonable trends reproduced. Finally, while at STP it has previously been shown that the solubility of CO2 is higher than that of He in NBR, we observe that under the right circumstances it is possible to reverse this trend.

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