

Electronic Supplementary Information

**Capture and immobilisation of Iodine (I₂) utilising
polymer-based ZIF-8 nanocomposite membranes**

*E. M. Mahdi, Abhijeet K. Chaudhuri, and Jin-Chong Tan**

*Department of Engineering Science, University of Oxford, Parks Road, OX1 3PJ,
Oxfordshire, United Kingdom*

*Email: jin-chong.tan@eng.ox.ac.uk

This supplementary document contains:

1. XRD diffractograms of the polymers and the nanocomposites	Fig. S1	p. 1
2. Chemical structure of Matrimid, PU, and ZIF-8	Fig. S2	p. 2
3. I ₂ release in EtOH and H ₂ O	Fig. S3	p. 3
4. Nanoindentation load-displacement data, averaged elastic moduli and hardness as a function of surface penetration depths of 2000 nm	Fig. S4	p. 4
5. Complete compilation of the TGA plots	Fig. S5	p. 5
6. Colour intensity change of PU/ZIF-8 nanocomposite with increasing filler wt.% loading	Fig. S6	p. 6

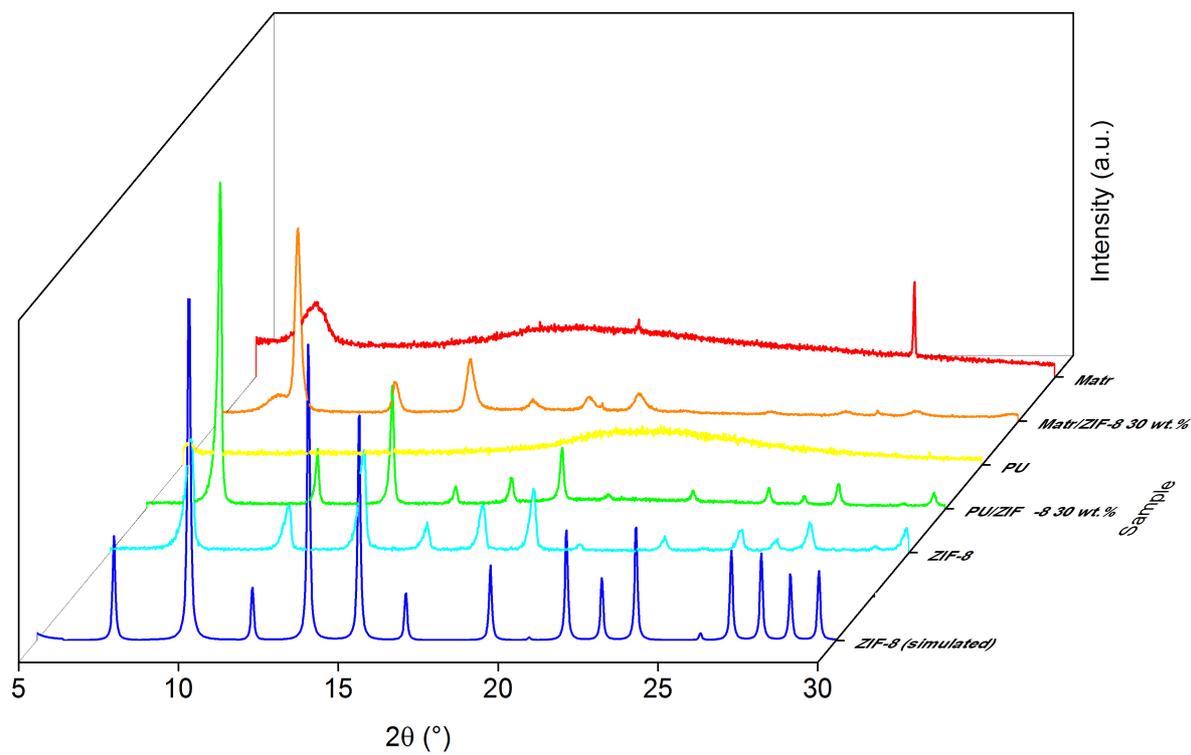


Figure S1. XRD of the polymers, ZIF-8 nanoparticles, its simulated pattern (from CSD Mercury v3.1), and the corresponding ZIF-8 nanocomposites

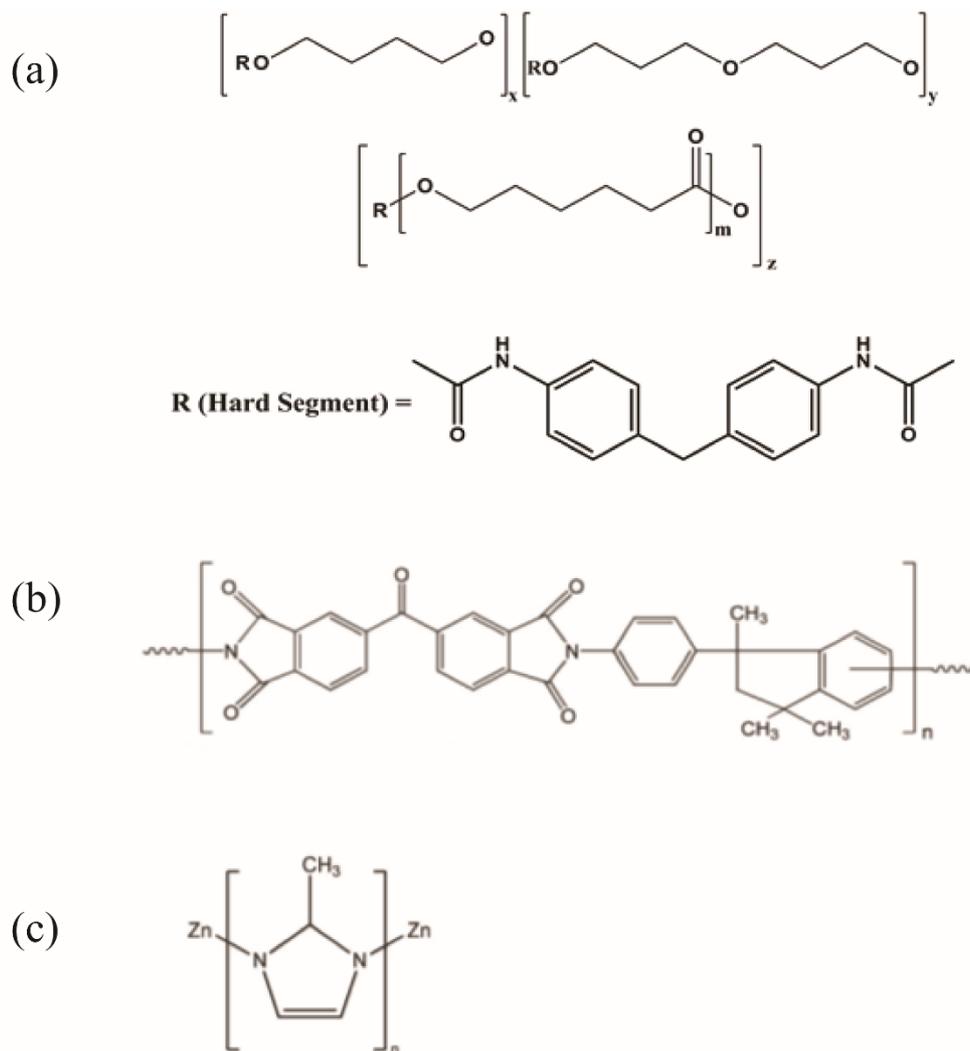


Figure S2. The chemical structures of the polymers and ZIF-8. Polyurethane (PU) is made up of hard and soft segments, as shown in (a), where the hard segments form bonds with other organic or organic based compounds. Matrimid is a glassy polymer, forming hard and very durable coating when dried. It is also made up of quite a few benzene rings, as shown in (b), which could form π - π bonds with ZIF-8, and (c) shows the chemical structure of ZIF-8, where the methyl group and the nitro group form bonds with the polymers when fabricating nanocomposites.

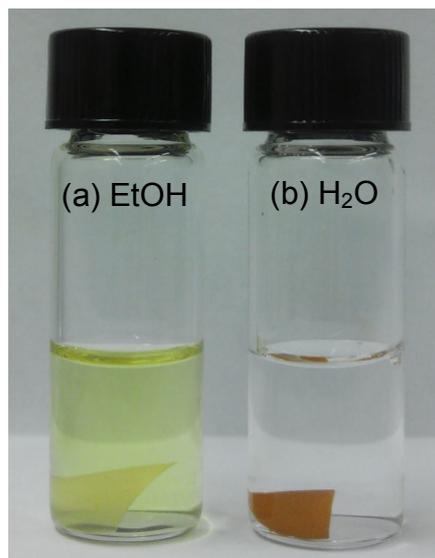


Figure S3. The vials above are of the PU/ZIF-8 30 wt.% I₂-adsorbed samples being set up for desorption experiments, with (a) EtOH (ethanol) medium, and (b) H₂O medium. The samples were left to desorb for 10 days, and after 10 days, the I₂ desorb into EtOH, but was completely retained in H₂O, with no signs of I₂ being released into H₂O. This proves that polarity of the medium is instrumental towards the release of I₂ from the nanocomposites, however, they remain stable in H₂O.

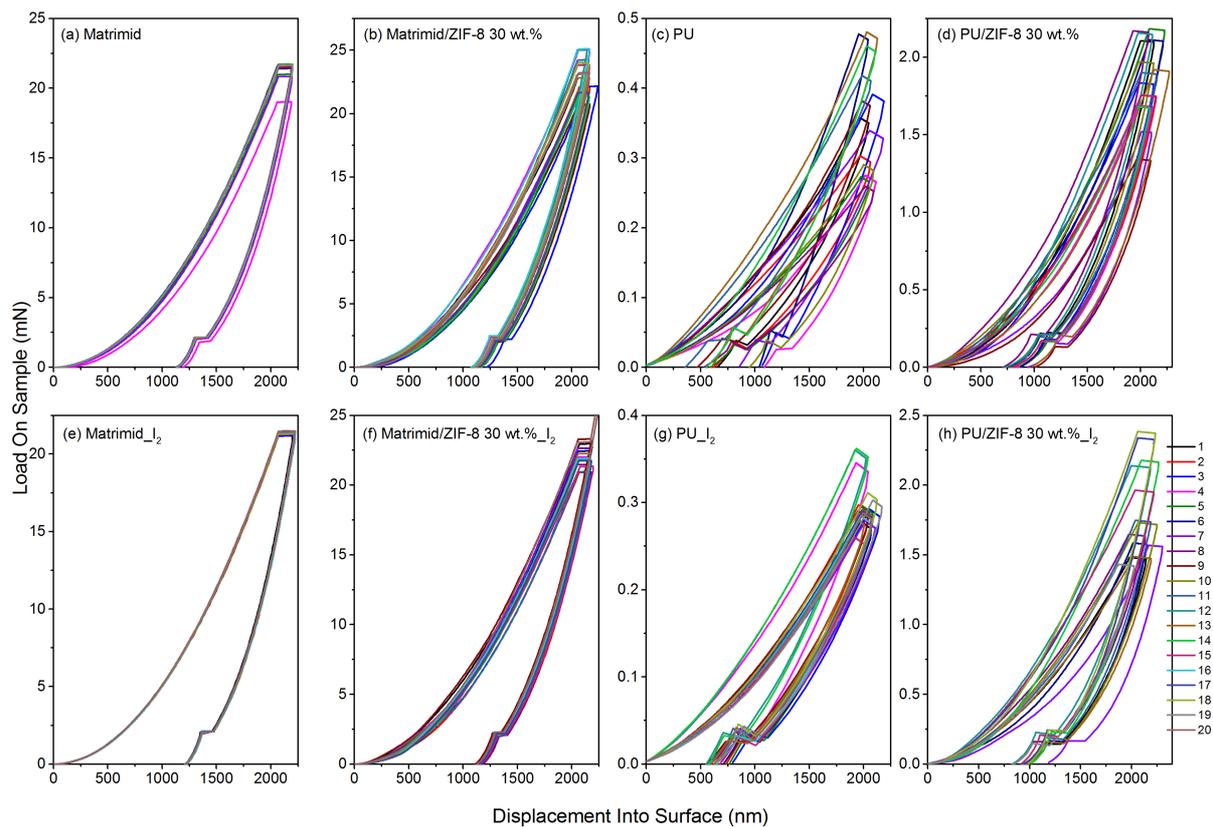


Figure S4. Nanoindentation load-displacement (P - h representative) plots for Matrimid, PU, and ZIF-8 nanocomposites, both blanks and loaded samples containing I_2 , with (a) Matrimid (blank), (b) Matrimid/ZIF-8 30 wt.% (blank), (c) PU (blank), (d) PU/ZIF-8 30 wt.% (blank), (e) Matrimid (I_2 absorbed), (f) Matrimid/ZIF-8 30 wt.% (I_2 absorbed), (g) PU (I_2 absorbed), (h) PU/ZIF-8 30 wt.% (I_2 absorbed). Note that the relatively higher scatter for the PU and PU nanocomposite could be attributed to the hyperelastic response of PU matrix.

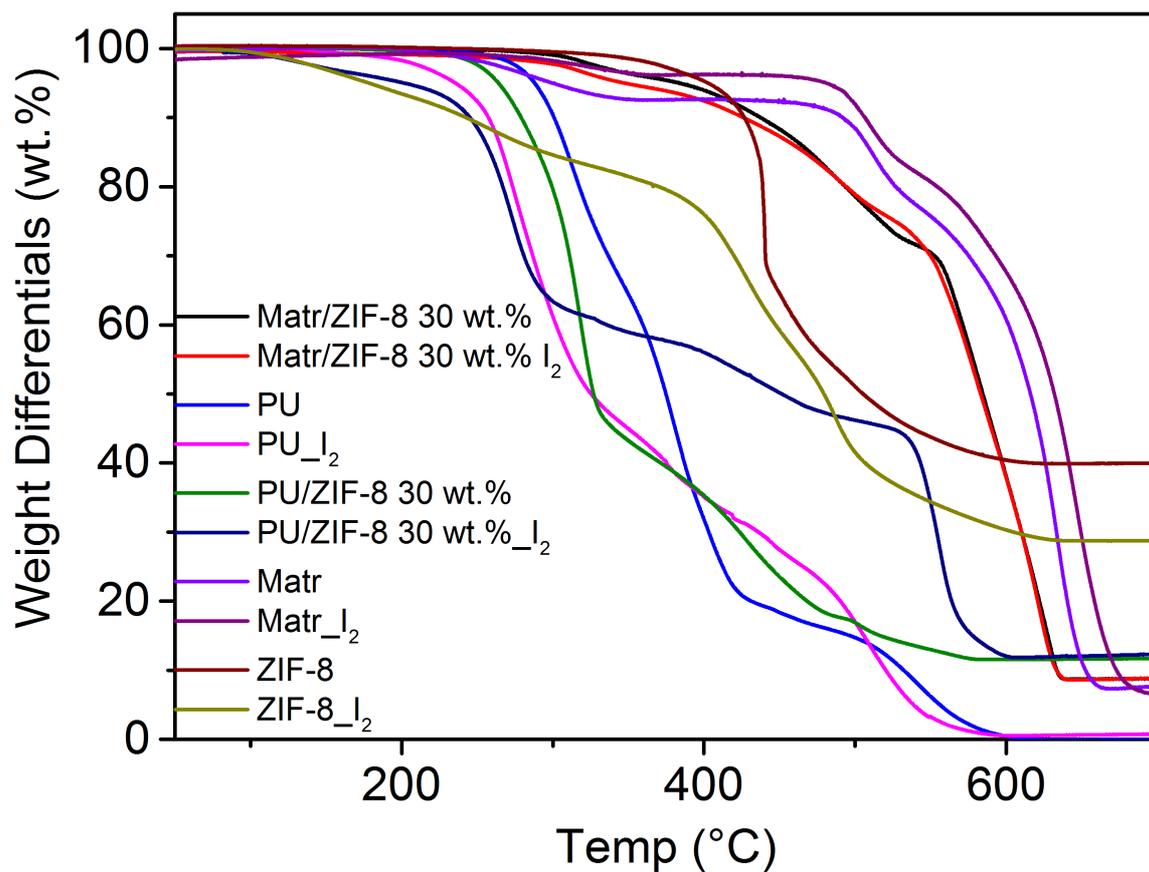


Figure S5. Compilation of the raw data pertaining to the TGA analyses of the polymers (PU, Matrimid), its nanocomposites (PU/ZIF-8 30 wt.% and Matr/ZIF-8 30 wt.%) and ZIF-8 nanoparticles pre- and post- I₂ absorption.

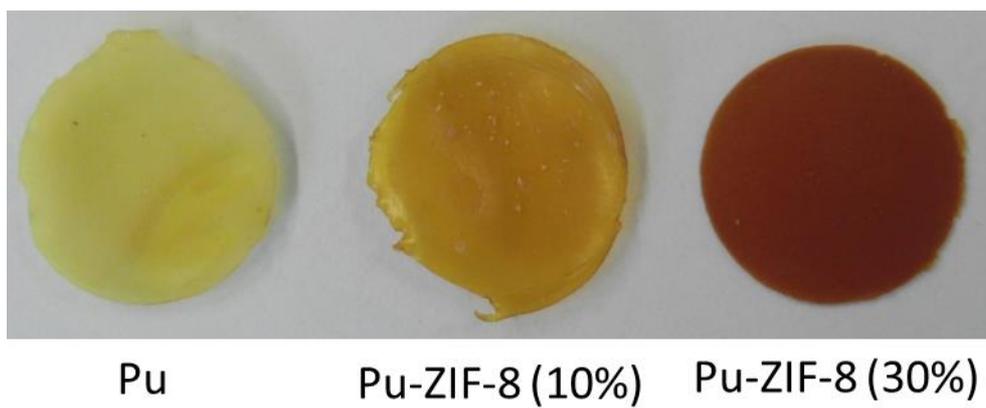


Figure S6. Effects of iodine capture in three PU-based membrane samples, showing the differing colouration intensity with an increasing MOF content from 0 to 30 wt.%.