Integrated approach for preventing hydrogen leakage from metallic vessels: barrier and scavenging

SUPPORTING INFORMATION

Yonatan Luzzatto, †[a] Amer Alatawna, †[a] Eli Peretz,[b] Orit Mendelson,[b] Svetlana Pevzner,[b] and Oren Regev[c]

The rate of 1,4-bis(phenylethynyl)benzene (PEB) hydrogenation is:

$$\frac{d[PEB]}{dt} = k\,(T)[PEB]^{X}[H_2]^{y} \quad \text{(S1)}$$

Where [PEB] is unsaturated concentration, *x* and *y* are the reaction orders, and *k(T)* is the temperature-dependent reaction constant. At a constant temperature and hydrogen pressure:

$$k_{obs} = k[H_2]^{y} \quad \text{(S2)}$$

Since the hydrogen pressure is constant during the experiment, and assuming a first-order reaction (*x*=1, approved experimentally, see Fig. S1), eqn S2 yields:

$$ln[PEB] = ln[PEB]_0 - k_{obs}t \quad \text{(S3)}$$

According to eqn S3, ln[PEB] shows a linear behavior with time, where the slope in the equation is the reaction constant (k_{obs}).

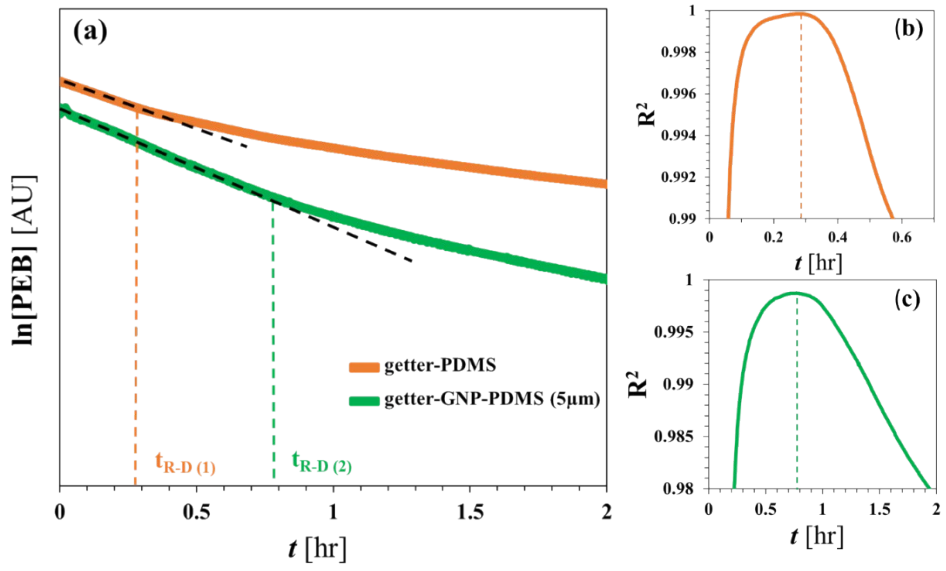

Fig. S1 (a) Reaction curves of getter-PDMS (orange) and getter-GNP-PDMS (green, 5 µm, 1 wt%). Dashed lines is a guid for the eye. The determination of $t_{R\text{-}D}$ was determined by following the change in the curve of R^2 vs. *t*. $t_{R\text{-}D}$ is the time at which the maximum R^2 is obtained, as shown for the getter-PDMS (b) and getter-GNP-PDMS systems (c).

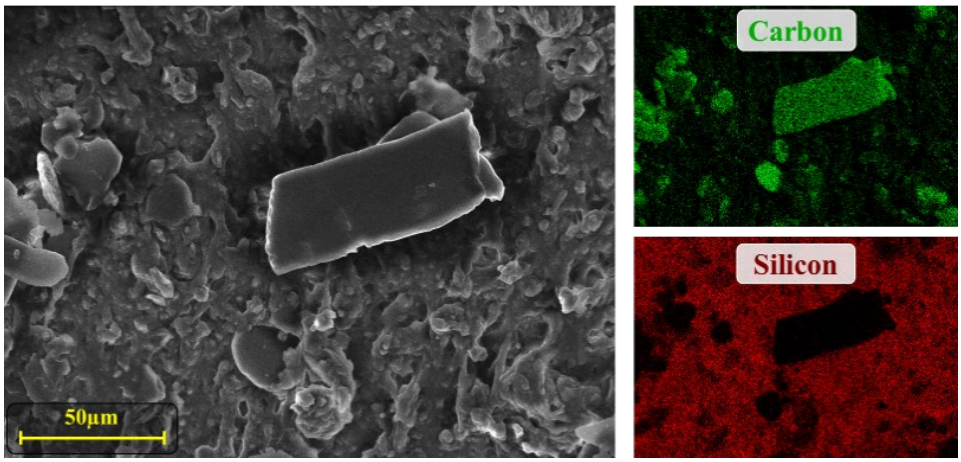

Fig. S2 EDS mapping of aggerates formed after hydrogenation at 296 K in a getter-PDMS system. A large aggregate was chosen (much above the average size) to simplify the analysis.

Element	Percentage
Carbon	81.7
Silicone	18.0
Palladium	0.1
Other	0.2

Table S1. Elemental analysis of the aggerates based on EDS (see Fig. S2).

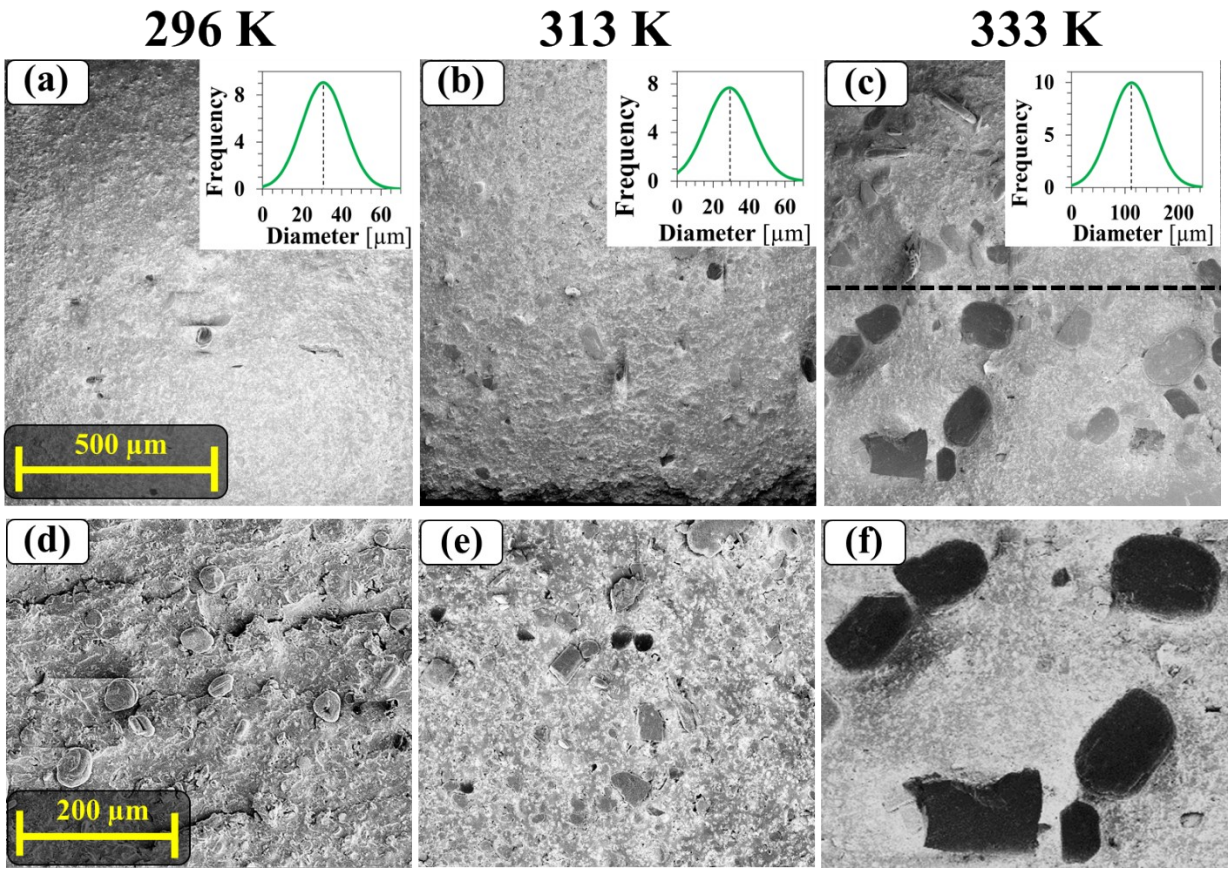

Fig. S3 A SEM micrograph of cross-sections in the **getter-GNP-PDMS** (5 μm GNP) system after hydrogenation at (a) 296 K, (b) 313 K: the aggregates were rather small (31± 11 μm and 29 ± 13 in size, n=50) and uniformly dispersed. (c) At 333 K, larger aggregates (112 ± 40 μm in size, n=50) were found at the bottom of the sample, most probably due to PEB liquefication followed by precipitation (delineated by a dashed line. Insets: size distributions of the aggregates. (d-f) higher magnification of the aggregates after hydrogenation at (d) 296 K, (e) 313 K, and (f) 333 K. In figures (a-c), the scalebar is 500 μm, and in (d-f), it is 200 μm.

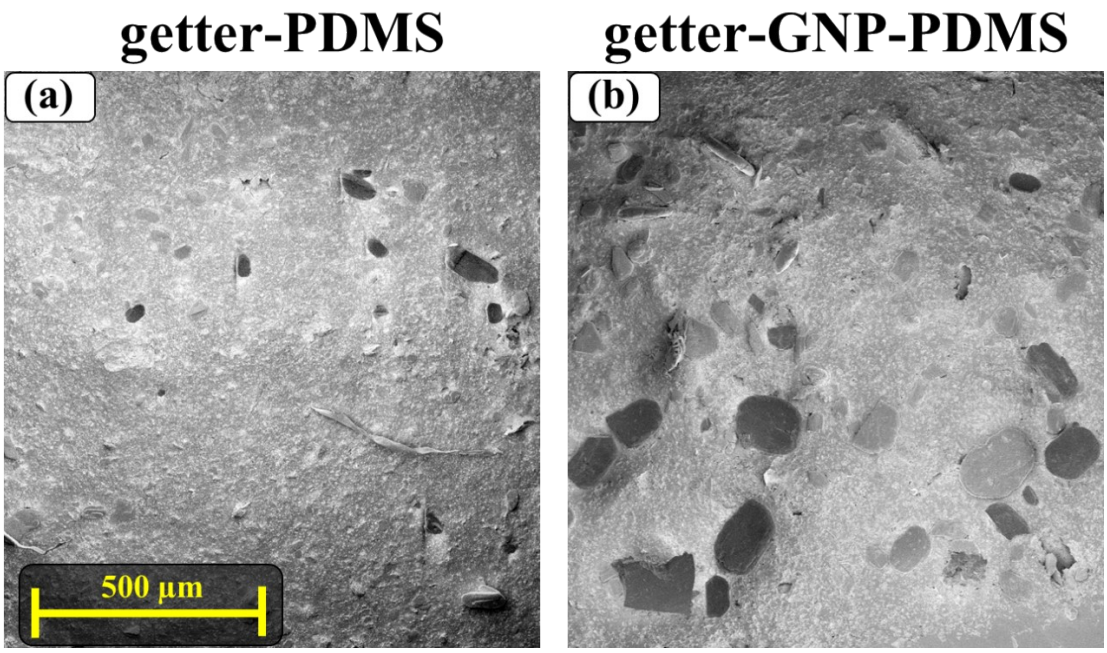

Fig. S4 Cross-sections of (a) getter-PDMS and (b) getter-GNP-PDMS system after hydrogenation at 333 K. The scale bar refers to both (a) and (b).

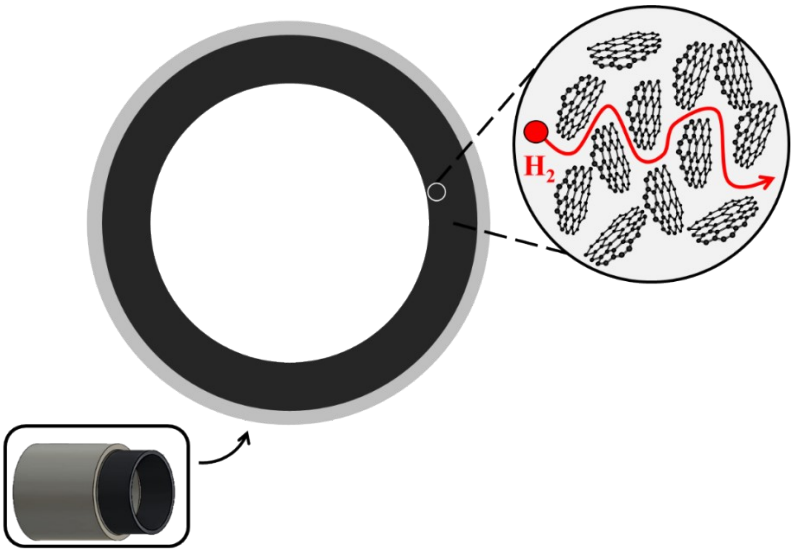

Fig. S5 A composite-based coating (polymer-GNP) created a tortuous path, decreasing hydrogen diffusion and, consequently, the composite permeability.

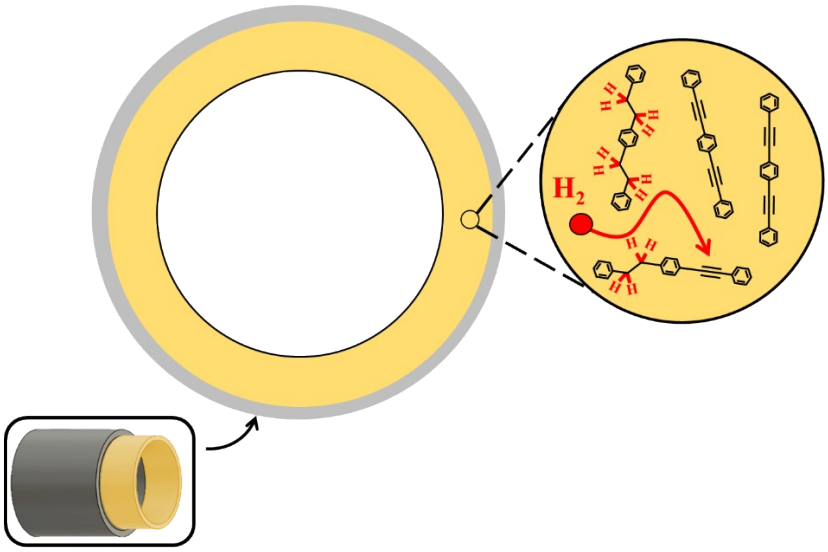

Fig. S6 A composite-based coating (polymer-PEB) that absorbed hydrogen, where unreacted and partially and fully hydrogenated PEB are shown. The red arrow symbols the reaction between hydrogen and the triple bond of a PEB molecule.

[a.] *Department of Chemical Engineering, Ben-Gurion University of the Negev, Beer-Sheva, 8410500 Israel.*
[b.] *c Department of Chemistry, Nuclear Research Centre-Negev, Beer-Sheva, 84190 Israel.*
[c.] *Department of Chemical Engineering Negev and Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Beer-Sheva, 8410500 Israel.*
† These authors were equally contributed to this article