Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary materials

Molecular simulations of gas transport in hydrogenated nitrile butadiene rubber and ethylene-propylene-diene rubber

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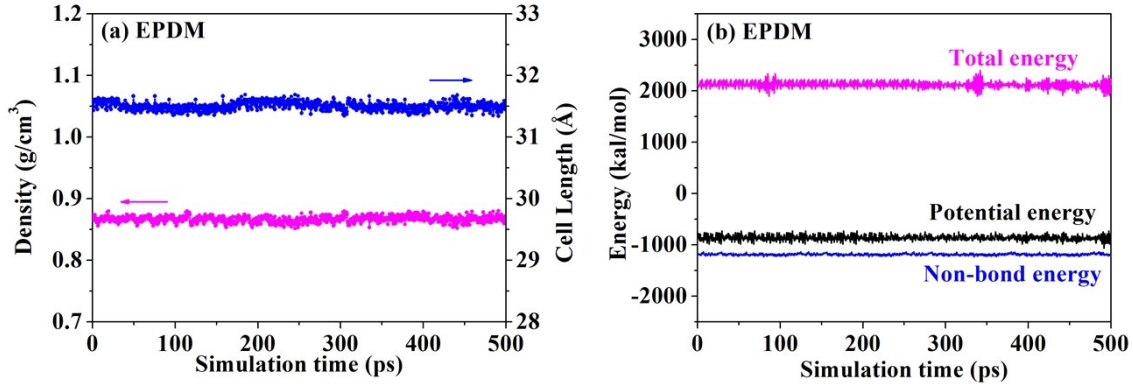


Fig. S1 Plots of (a) density, cell length and (b) energy versus simulation time in the NPT simulation for EPDM.

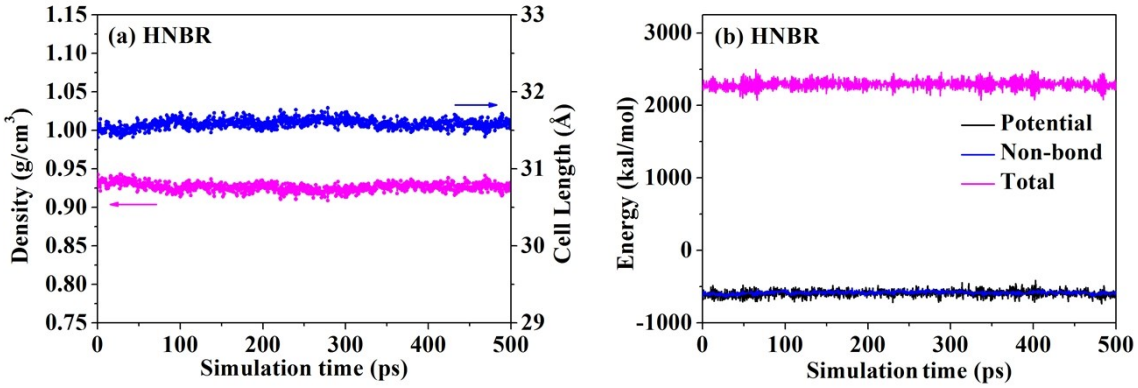


Fig. S2 Plots of (a) density, cell length and (b) energy versus simulation time in the NPT simulation for HNBR.

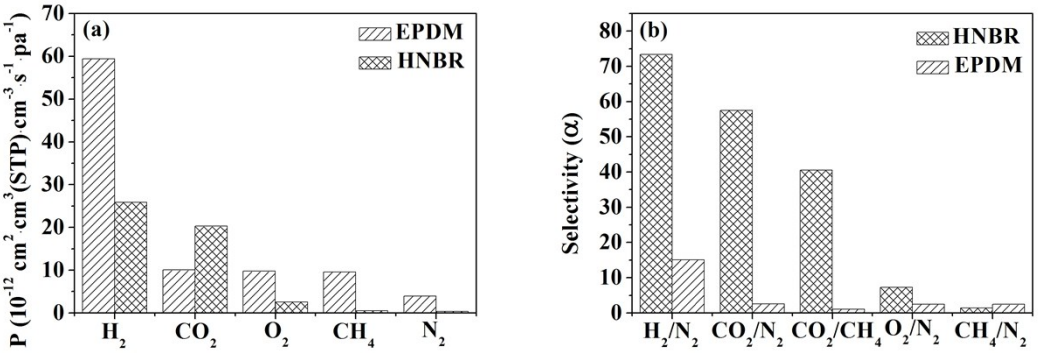
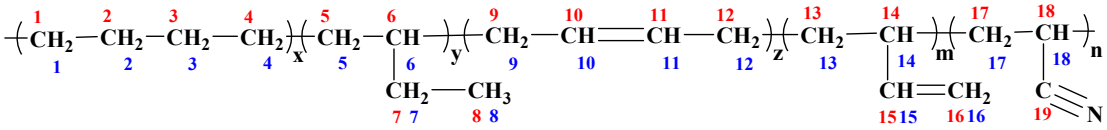
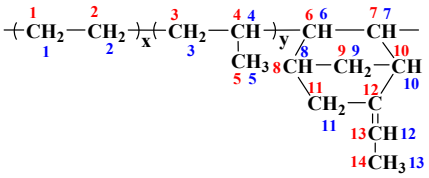


Fig. S3 The (a) permeabilty coefficients and (b) selectivity of penetrant molecules in HNBR and EPDM

Table S1 Non-bonded force field parameters for the EPDM and HNBR



Atom	*q* (e)	Force field type
C1/C2/C3/C4/C5/C7/C9/C12/C13/C17	-0.106	c4
C6/C14	-0.053	c43
C8	-0.159	c4
C10/C11/C15	-0.127	c3=
C16	-0.254	c3=
C18	0.141	c43
C19	0.234	c2t
H1/H2/H3/H4/H5/H6/H7/H8/H9	0.053	h1
H12/H13/H14/H17/H18		
H10/H11/H15/H16	0.127	h1
N	-0.428	n1t



C1/C2/C3	-0.106	c4
C4/C6/C7/C8/C10	-0.053	c43
C5/C14	-0.159	c4
C9/C11	-0.106	C4
C12	0	c3=
C13	-0.127	c3=
H1/H2/H3/H4/H5/H6	0.053	h1
H7/H8/H9/H10/H11/H13		
H12	0.127	h1