Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information

Strain-Induced Geometric Modulation of Nanopores for Enhanced Hydrogen Isotopologue Separation via Quantum Sieving

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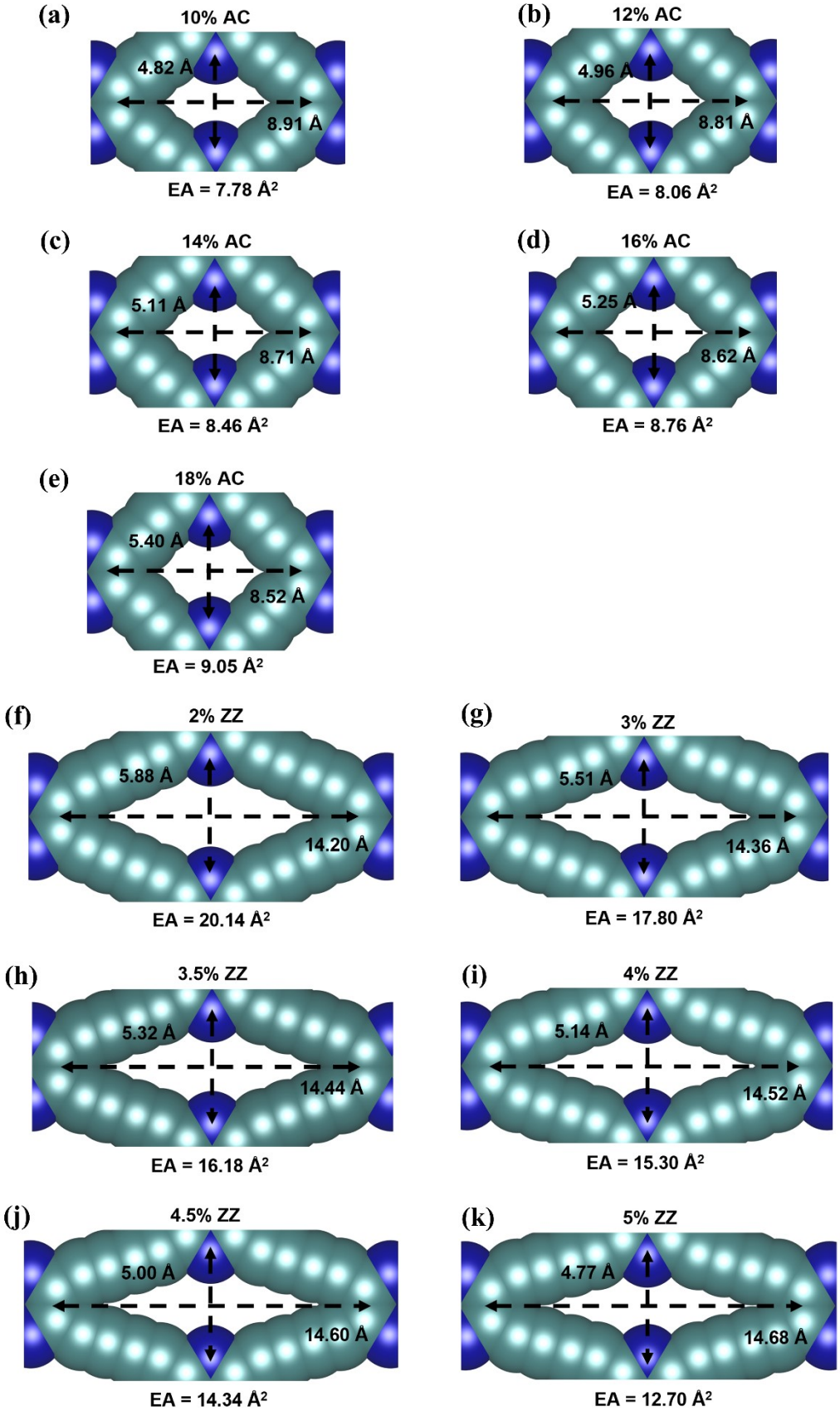
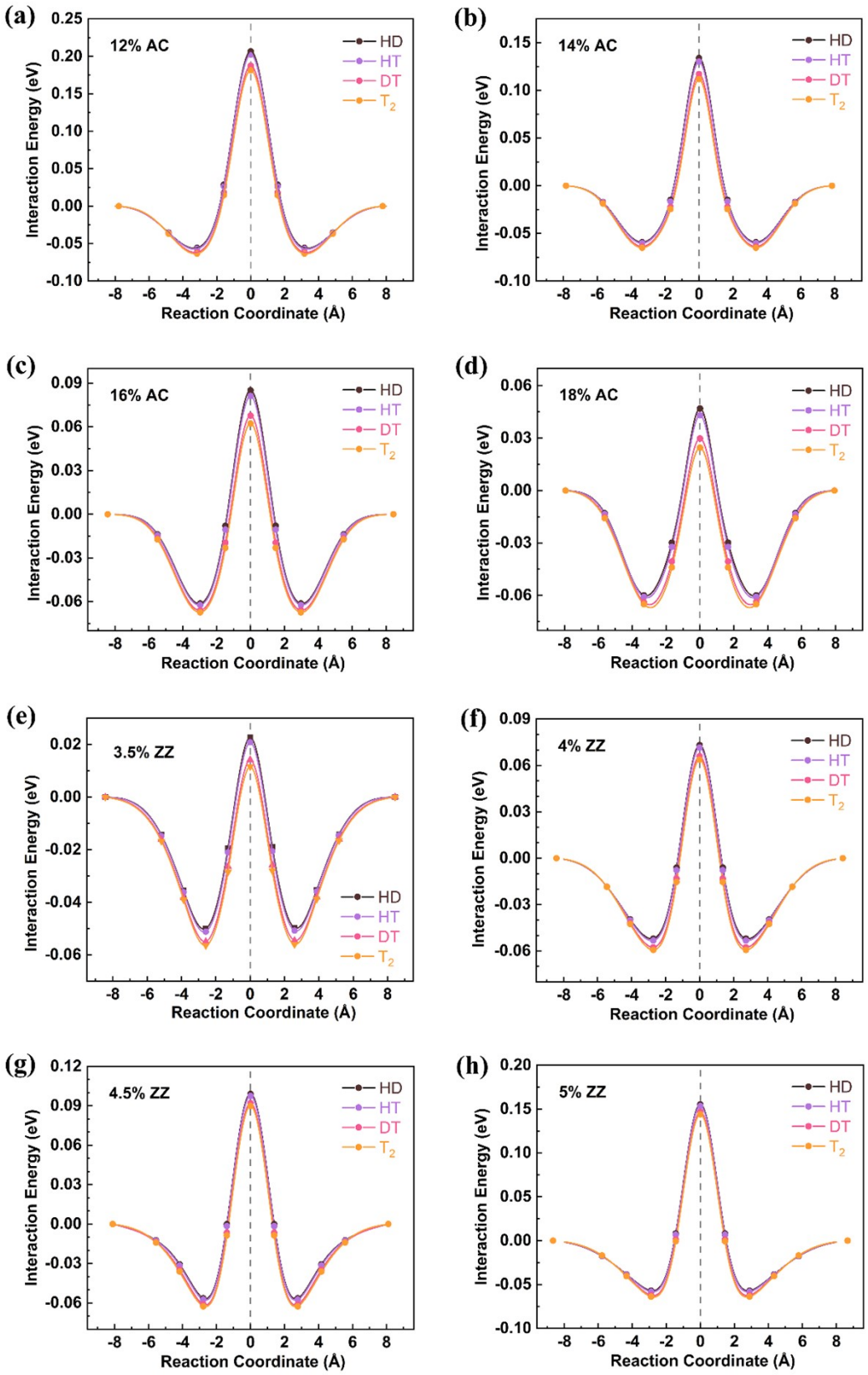
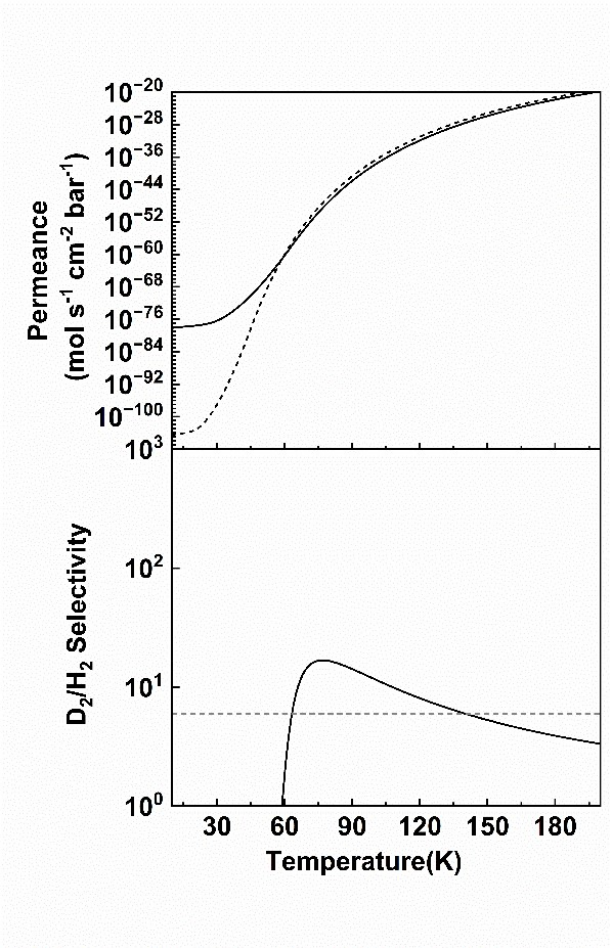


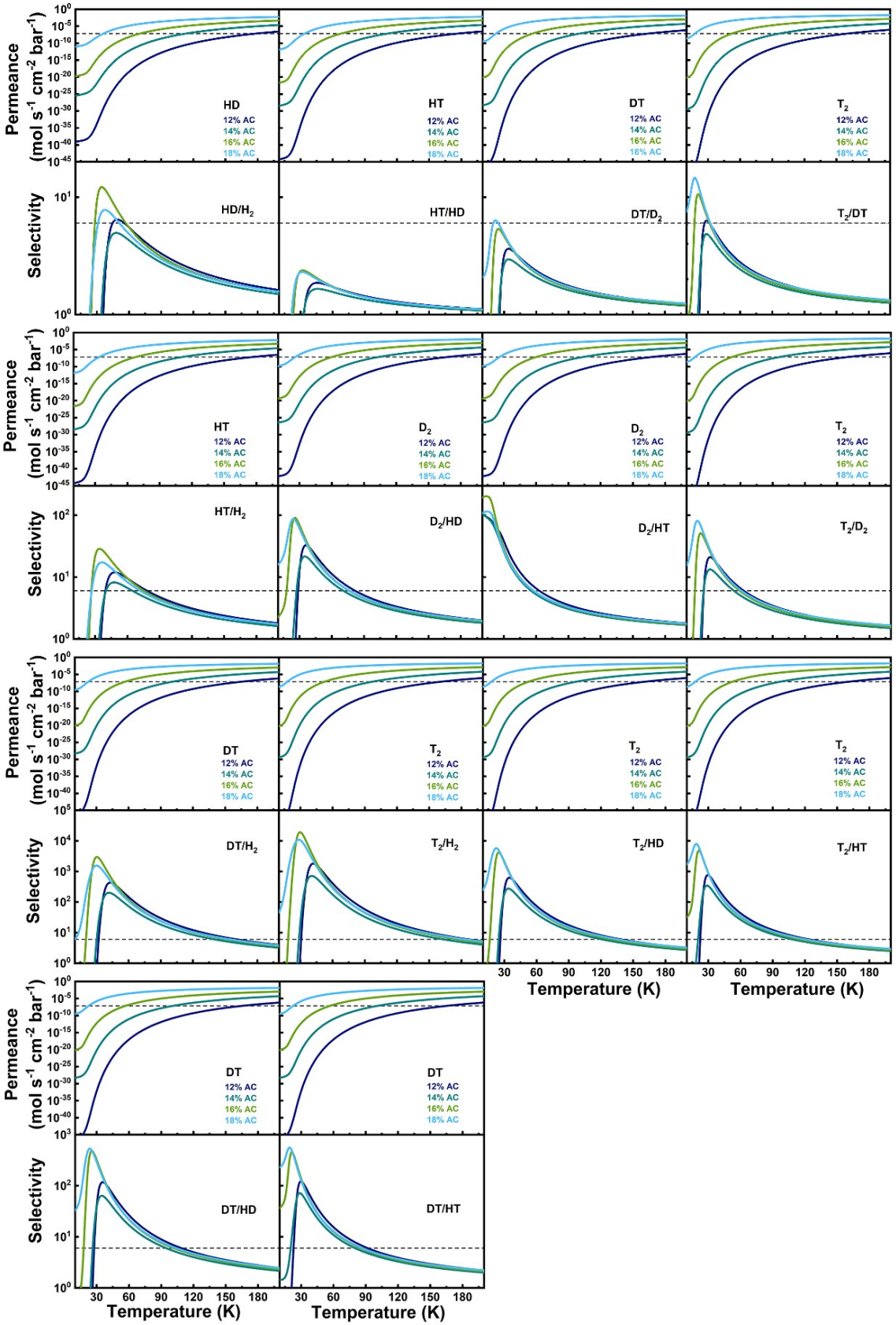
Figures S1. Geometric evolution of the nanopores in *r*-N-GY (a)-(e) and *r*-N-GDY (f)-(k) membranes under different strains.



Figures S2. ZPE-corrected energy profiles of hydrogen isotopologues passing through strained nanopores. (a)-(d) 12%-18% AC-strained *r*-N-GY nanopores. (e)-(h) 3.5%-5% ZZ-strained *r*-N-GDY nanopores.



Figures S3. H_2 (solid line) and D_2 (dashed line) permeance and D_2/H_2 selectivity for the unstrained *r*-N-GY membrane over 10-200 K. Gray dashed line in the lower panel indicates industrial selectivity threshold of 6.



Figures S4. Permeance and selectivity of hydrogen isotopologues through 12%-18% AC-strained *r*-N-GY membranes across 10-200 K. Gray dashed lines indicate industrial standards: upper (permeance threshold: 6.7×10^{-8} mol s^{-1} cm^{-2} bar^{-1}) and lower (selectivity threshold: 6).

Table S1 Atomic coordinates of unstrained *r*-N-GY.

Spce group: CMMM (D2H-19) **a = 11.60 Å, b = 6.92 Å, and c = 30.00 Å** **α = 90°, β = 90°, and γ = 90°**			
	X	**Y**	**Z**
C	0.159580007	0.352589995	0.494320005
C	0.159590006	0.560790002	0.494289994
C	0.264230013	0.248659998	0.494309992
C	0.264259994	0.664600015	0.494300008
C	0.461409986	0.060800001	0.494280007
C	0.461409986	0.852599978	0.494300008
C	0.356730014	0.164580002	0.494289994
C	0.356759995	0.748690009	0.494280007
C	0.659590006	0.060800001	0.494289994
C	0.659590006	0.852590024	0.494320005
C	0.764259994	0.164609998	0.494300008
C	0.764219999	0.748640001	0.494309992
C	0.856750011	0.248699993	0.494280007
C	0.856729984	0.664569974	0.494289994
C	0.961419999	0.352600008	0.494300008
C	0.961419999	0.560790002	0.494280007
N	0.060499999	0.252119988	0.494320005
N	0.060499999	0.661289989	0.494300008
N	0.560500026	0.161269993	0.494300008
N	0.560500026	0.752129972	0.494320005

Table S2 Atomic coordinates of unstrained *r*-N-GDY.

Spce group: CMMM (D2H-19) **a = 16.18 Å, b = 9.28 Å, and c = 30.00 Å** **α = 90°, β = 90°, and γ = 90°**			
	X	**Y**	**Z**
C	0.071587288	0.424353397	0.500081778
C	0.071563064	0.580091172	0.500046194
C	0.146738564	0.348141080	0.500117123
C	0.146655006	0.656574743	0.500060916
C	0.214053656	0.286722983	0.500112712
C	0.213775047	0.718627266	0.500042677
C	0.287336996	0.218996204	0.500063300
C	0.287044466	0.786454565	0.500007749
C	0.354388882	0.156715866	0.499986440
C	0.354254200	0.848188728	0.499956518
C	0.429409735	0.080157634	0.499926120
C	0.429384526	0.924424472	0.499923617
C	0.571618904	0.080081153	0.499916285
C	0.571620666	0.924380011	0.499917060
C	0.646681174	0.156570939	0.499931216
C	0.646734385	0.848067356	0.499940217
C	0.713742294	0.218781145	0.499989629
C	0.713982132	0.786430909	0.499971151
C	0.786969411	0.286672702	0.500023782
C	0.787190480	0.718468898	0.499997646
C	0.854248262	0.348162258	0.500037968
C	0.854282108	0.656319569	0.500004649
C	0.929408228	0.424298971	0.500036895
C	0.929380507	0.579984971	0.500014484
N	0.000510348	0.349286697	0.500070989

N	0.000461662	0.655067695	0.500012994
N	0.500540233	0.155090244	0.499903083
N	0.500503997	0.849444061	0.499906719