

Electronic Supplementary Information

to

Transport properties of thermoplastic R-BAPB polyimide: molecular-dynamics simulations and experiment

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Table S1. Properties of R-BAPB thin film membrane considered in the work.

T_g , K	T_m , K	τ_5 , K	σ , MPa	E , MPa	ϵ , %
485	599	805	108.4±13.5	2514±104	95.2±33.2
T_g – glass transition temperature, T_m – melting temperature, τ_5 – decomposition temperature, σ – tensile strength, E – elasticity modulus, ϵ – tensile strain.					

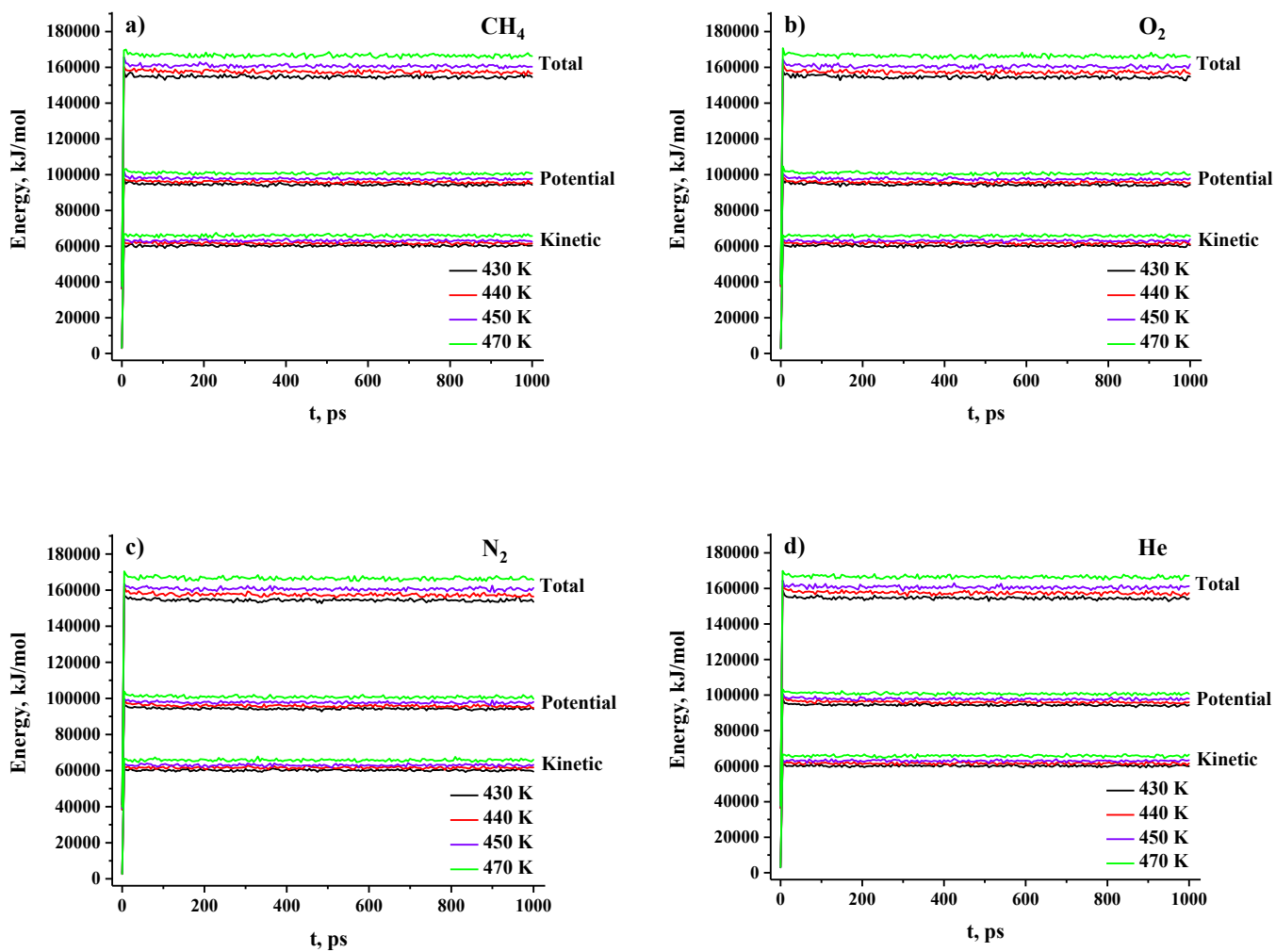


Figure S1. Time dependence of the potential, kinetic and total energies of R-BAPB sample containing a) CH₄, b) O₂, c) N₂, or d) He at different temperatures after energy minimization.

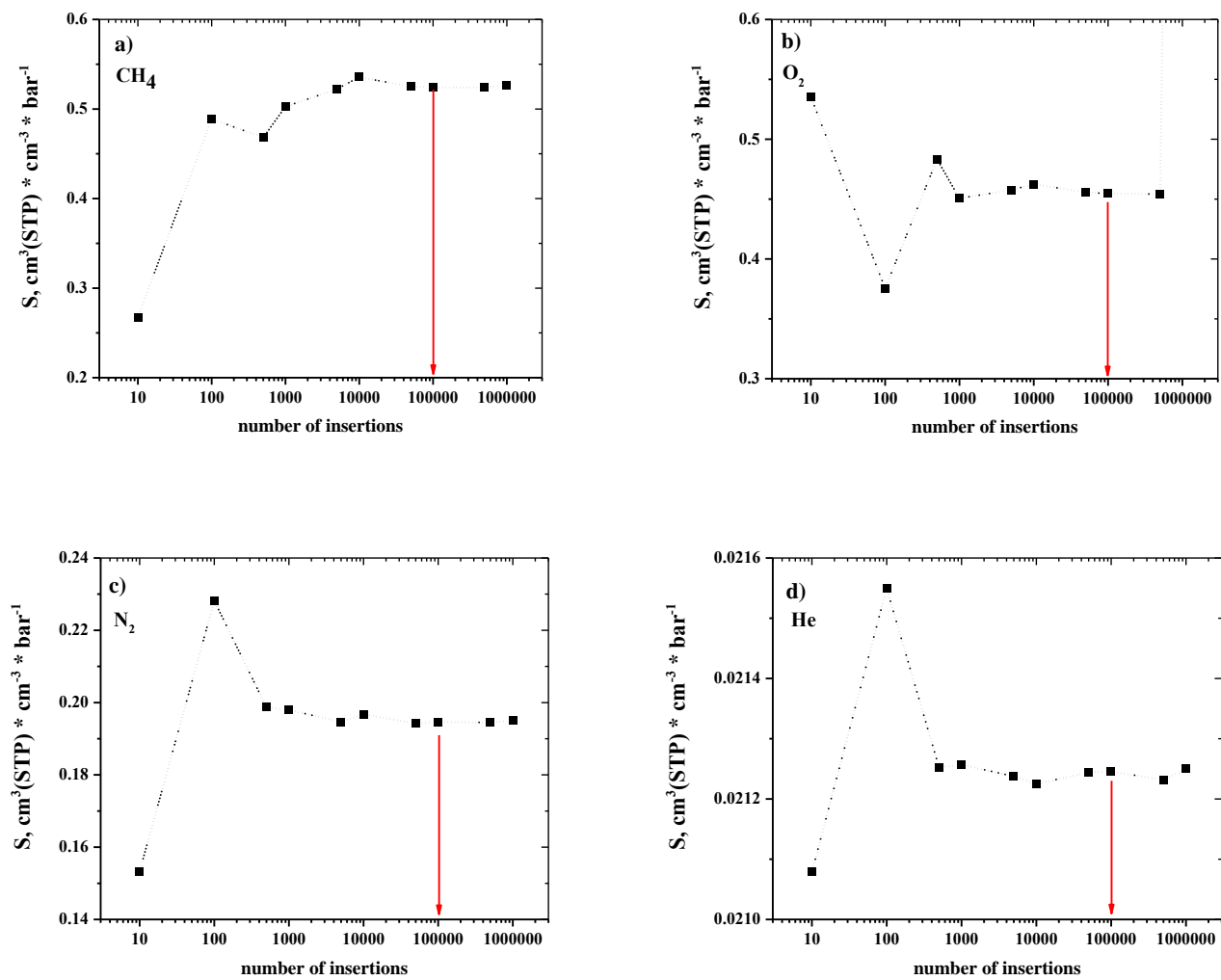


Figure S2. Dependence of the solubility coefficient of a) CH₄, b) O₂, c) N₂, or d) He at STP conditions calculated from a single trajectory obtained at $T = 300$ K on the number of the test particle insertions. The arrow denotes an optimal number of insertions ($n = 100,000$).

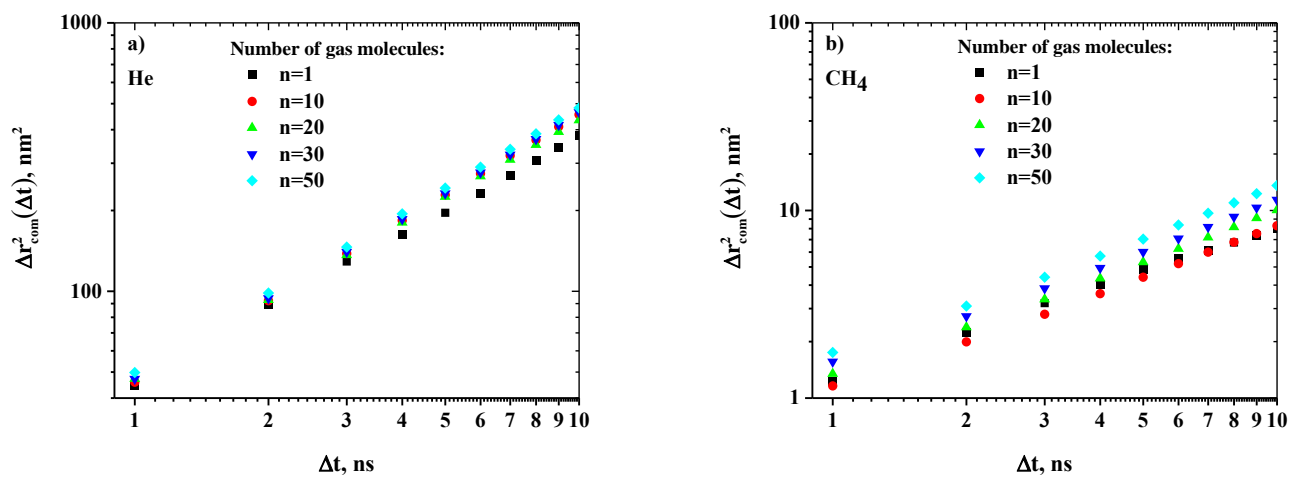


Figure S3. Time-dependence of mean squared displacement of a) He or b) CH_4 gas molecules in R-BAPB at different concentrations (number of gas molecules in the system) at $T = 470$ K calculated over 100 ns.

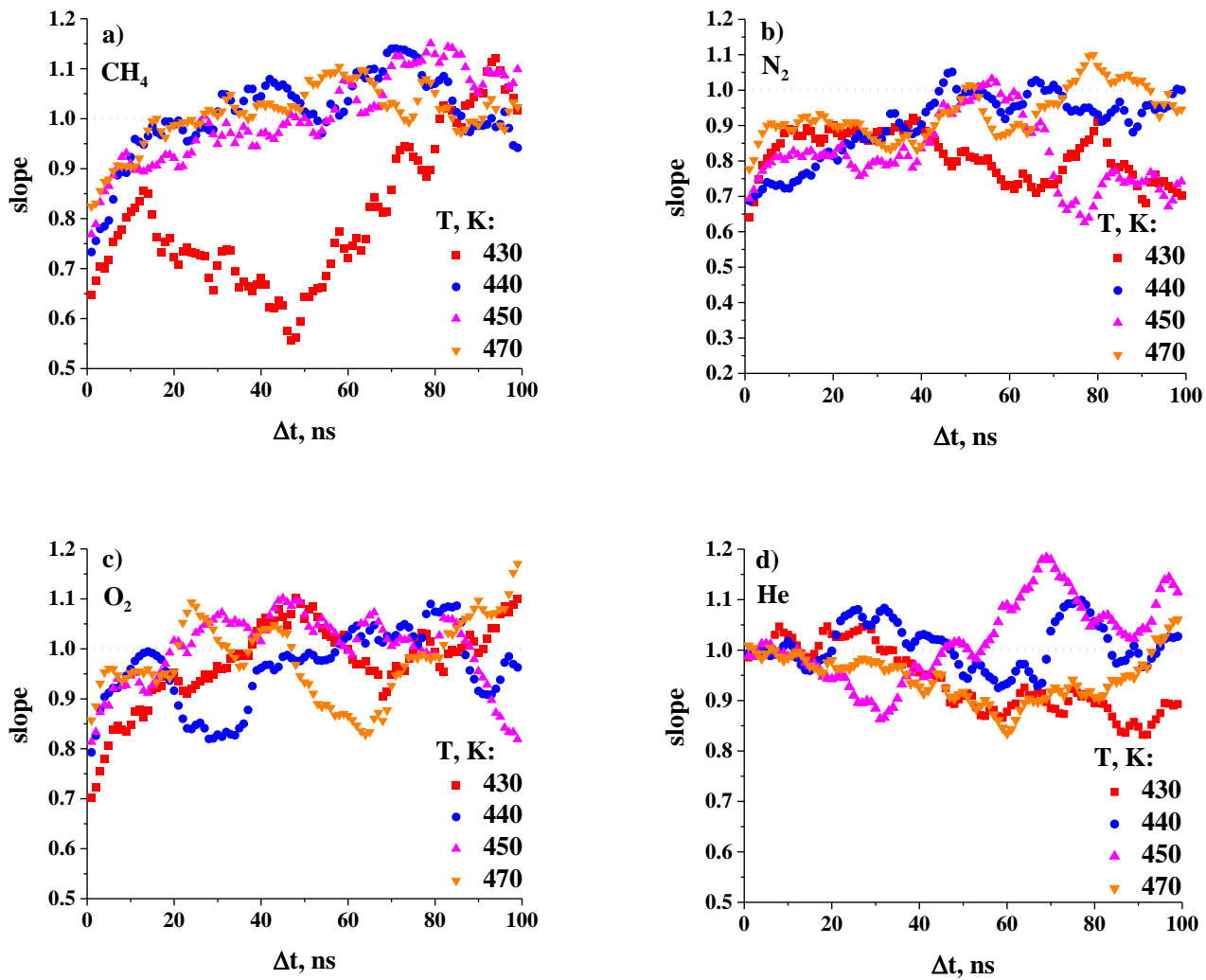


Figure S4. Time-dependence of the slope of the mean squared displacement of a) CH₄, b) O₂, c) N₂, or d) He gas molecules in R-BAPB at different temperatures (the number of gas molecules in the system is equal 10).