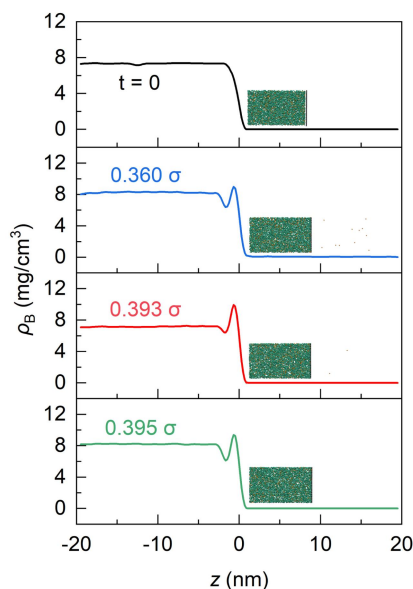
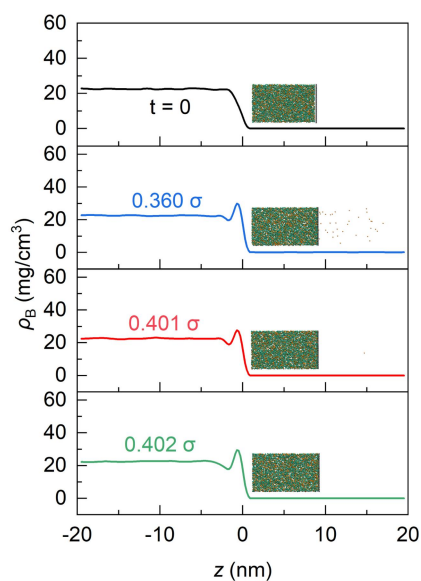


# Molecular Simulations of the Gas Diffusion through the Two-dimensional Graphyne Membrane

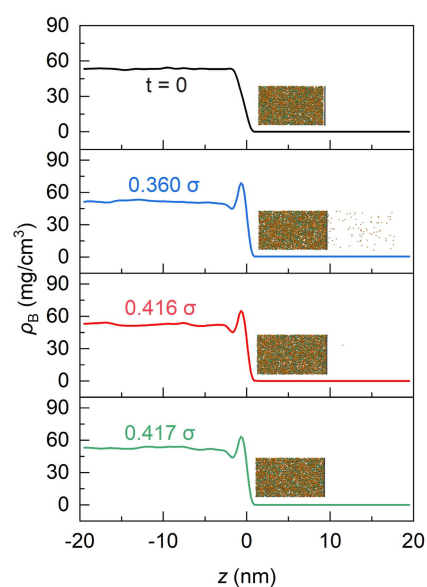
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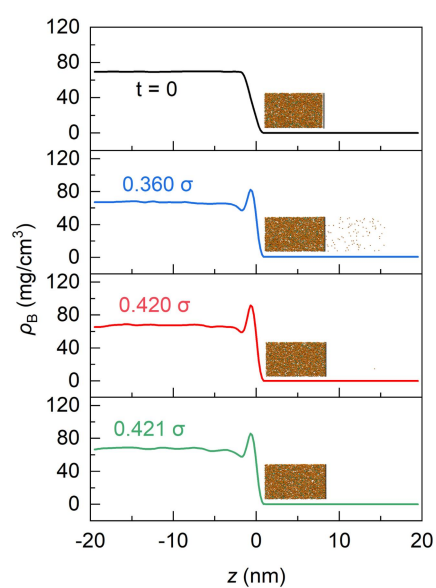
**Figure S1.** Density  $\rho_B$  of the species B as a function of the  $z$  coordinates for temperature  $T = 300$  K under partial pressure difference  $\Delta p_B = 9$  bar (total pressure difference  $\Delta p = 95$  bar, initial total density  $\rho = 80$  mg/cm<sup>3</sup>, and mole fraction of the species  $x_B = 0.1$ ).



**Figure S2.** Density  $\rho_B$  of the species B as a function of the  $z$  coordinates for temperature  $T = 300$  K under partial pressure difference  $\Delta p_B = 28$  bar (total pressure difference  $\Delta p = 95$  bar, initial total density  $\rho = 80$  mg/cm<sup>3</sup>, and mole fraction of the species  $x_B = 0.3$ ).



**Figure S3.** Density  $\rho_B$  of the species B as a function of the z coordinates for temperature  $T = 300$  K under partial pressure difference  $\Delta p_B = 66$  bar (total pressure difference  $\Delta p = 95$  bar, initial total density  $\rho = 80$  mg/cm<sup>3</sup>, and mole fraction of the species  $x_B = 0.7$ ).



**Figure S4.** Density  $\rho_B$  of the species B as a function of the z coordinates for temperature  $T = 300$  K under partial pressure difference  $\Delta p_B = 85$  bar (total pressure difference  $\Delta p = 95$  bar, initial total density  $\rho = 80$  mg/cm<sup>3</sup>, and mole fraction of the species  $x_B = 0.9$ ).