

Supplementary information

Decomposition of CH₄ hydrate: effects of temperature and salt from molecular simulations

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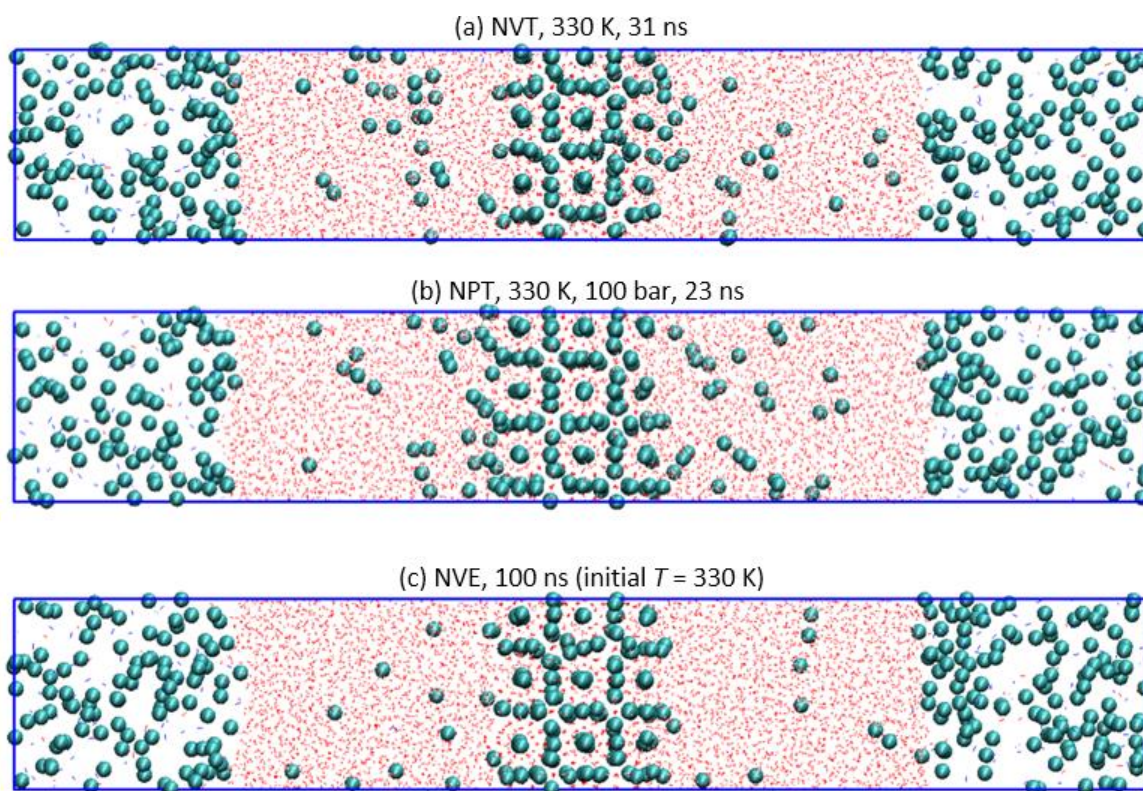


Figure S1. Simulation snapshots in three ensembles (NVT, NPT and NVE).

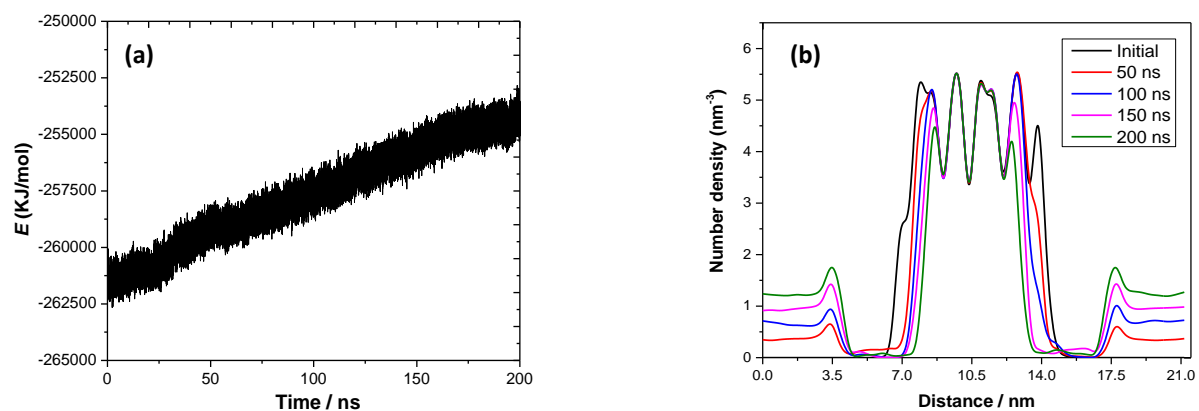


Figure S2. Decomposition at 300 K (a) potential energy (b) density profiles of CH₄ along the x -axis.

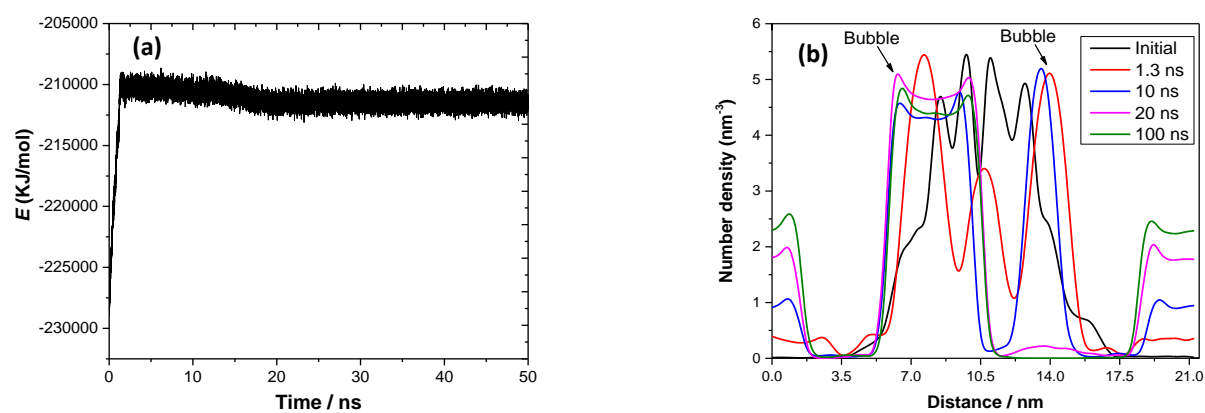


Figure S3. Decomposition at 360 K (a) potential energy (b) density profiles of CH₄ along the x -axis.

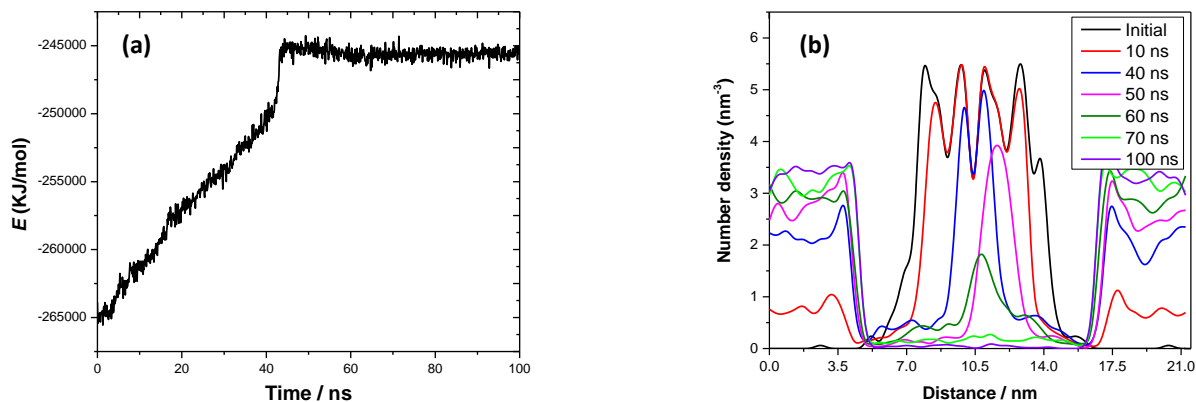


Figure S4. Decomposition at 330 K with 0.6 M NaCl (a) potential energy (b) density profiles of CH₄ along the x -axis.

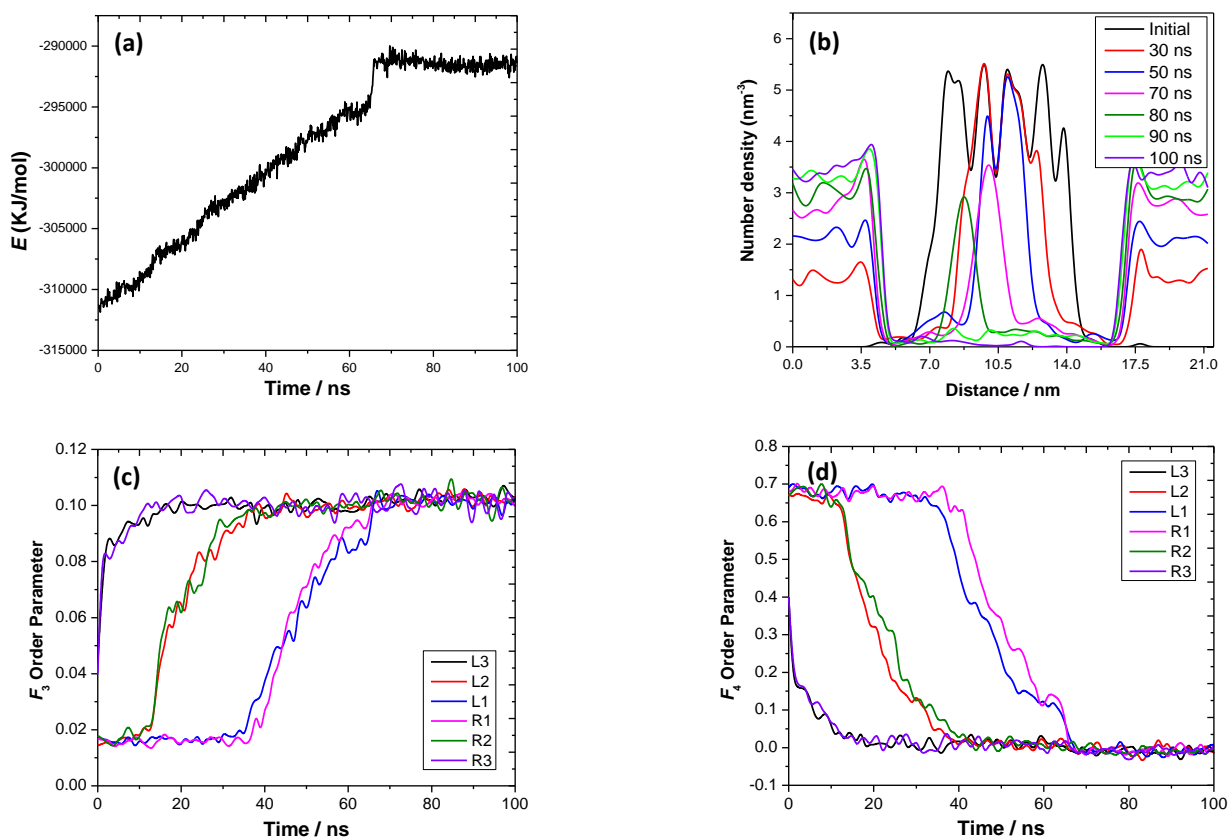


Figure S5. Decomposition at 330 K with 1.8 M NaCl (a) potential energy (b) density profiles of CH₄ along the x -axis (c) F_3 and (d) F_4 parameters in different layers.

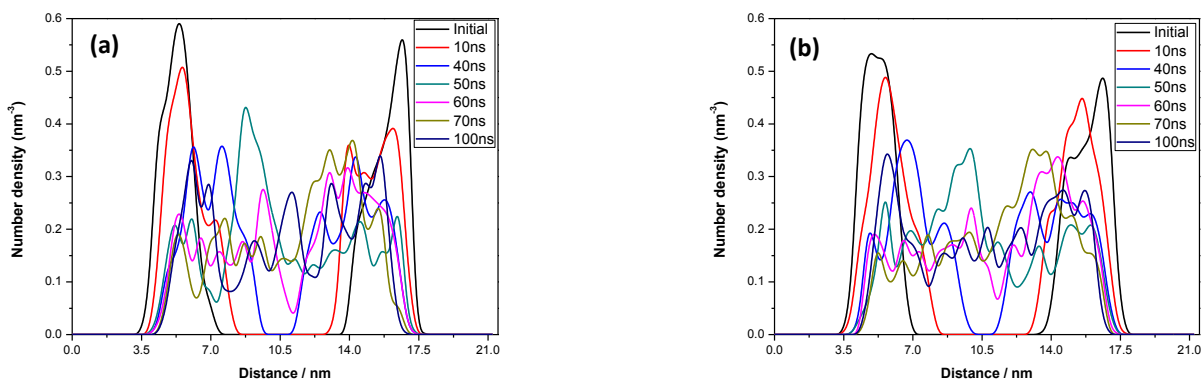


Figure S6. Density profiles of (a) Na⁺ and (b) Cl⁻ along the x -axis at 330 K with 0.6 M NaCl.

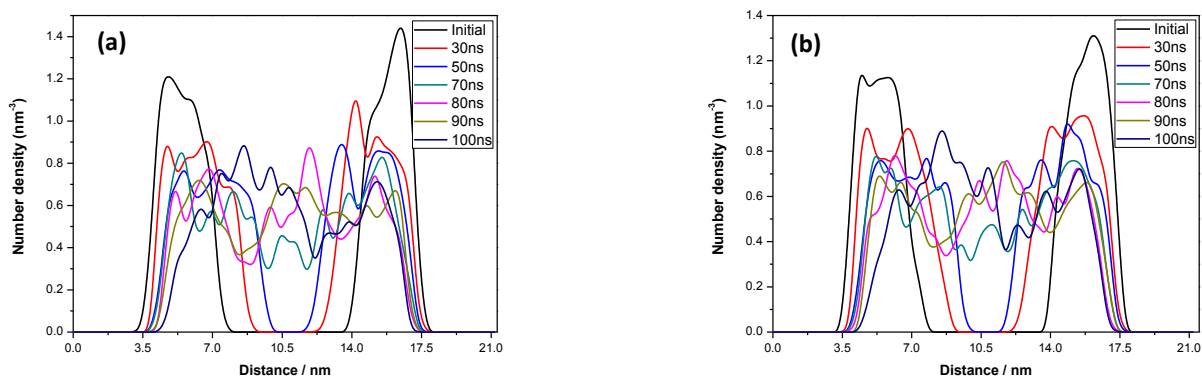


Figure S7. Density profiles of (a) Na⁺ and (b) Cl⁻ along the x -axis at 330 K with 1.8 M NaCl.

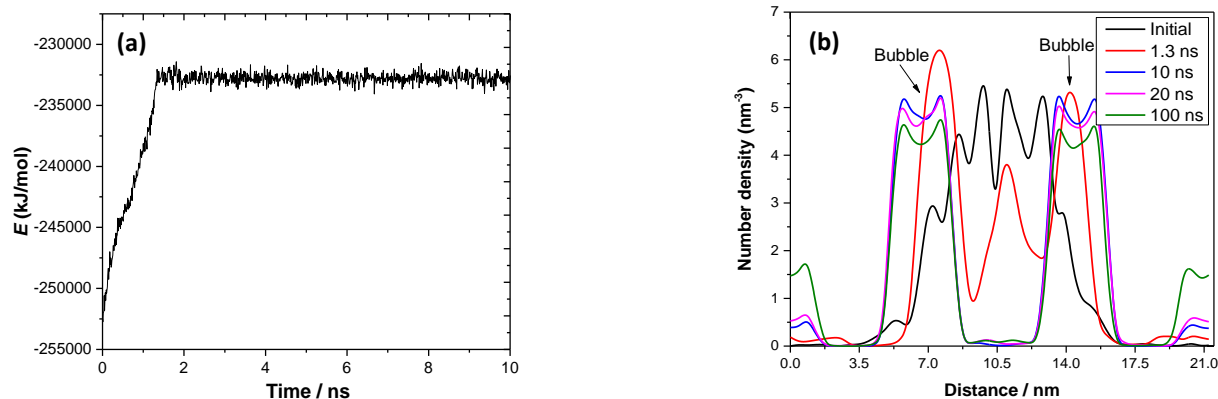


Figure S8. Decomposition at 360 K with 0.6 M NaCl (a) potential energy (b) density profiles of CH₄ along the x -axis.

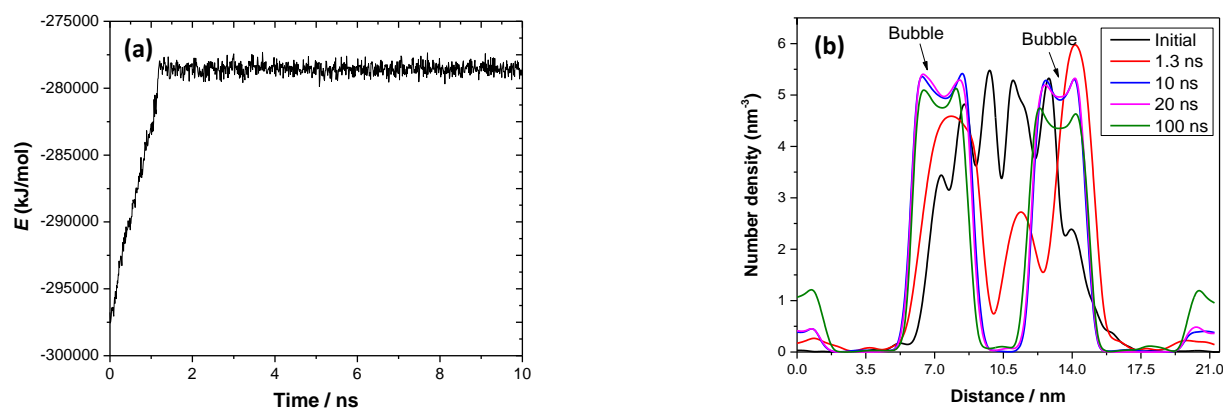


Figure S9. Decomposition at 360 K with 1.8 M NaCl (a) potential energy (b) density profiles of CH₄ along the x -axis.