

Supporting information for:

Reaction Coordinate of Incipient Methane Clathrate Hydrate Nucleation

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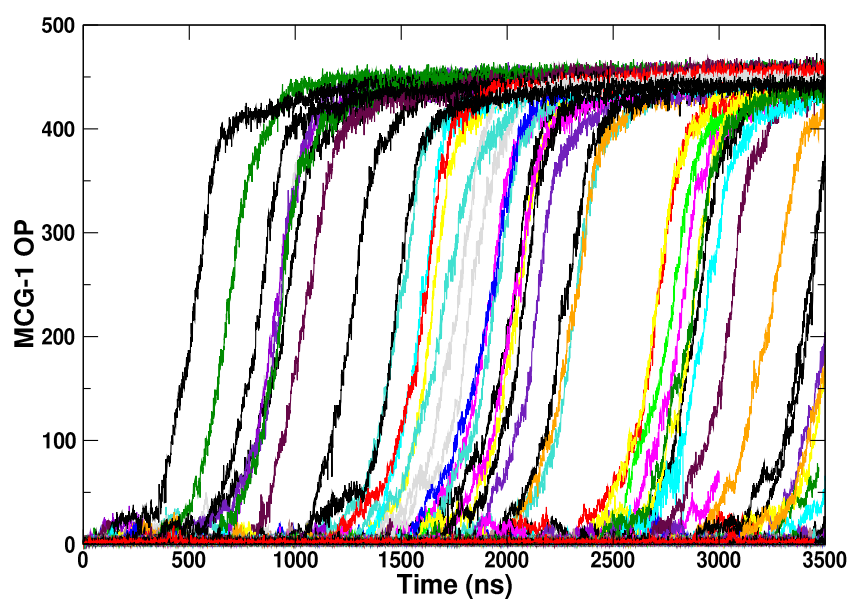


Figure S1: MCG-1 results for 200 multi-microsecond MD trajectories at $P = 500$ bar, $T = 255$ K. At the plateau for MCG-1 values in the mid-400s, hydrate is spanning the entire simulation cell in all directions and the gas phase is essentially depleted. The variation in induction times is consistent with a stochastic process.

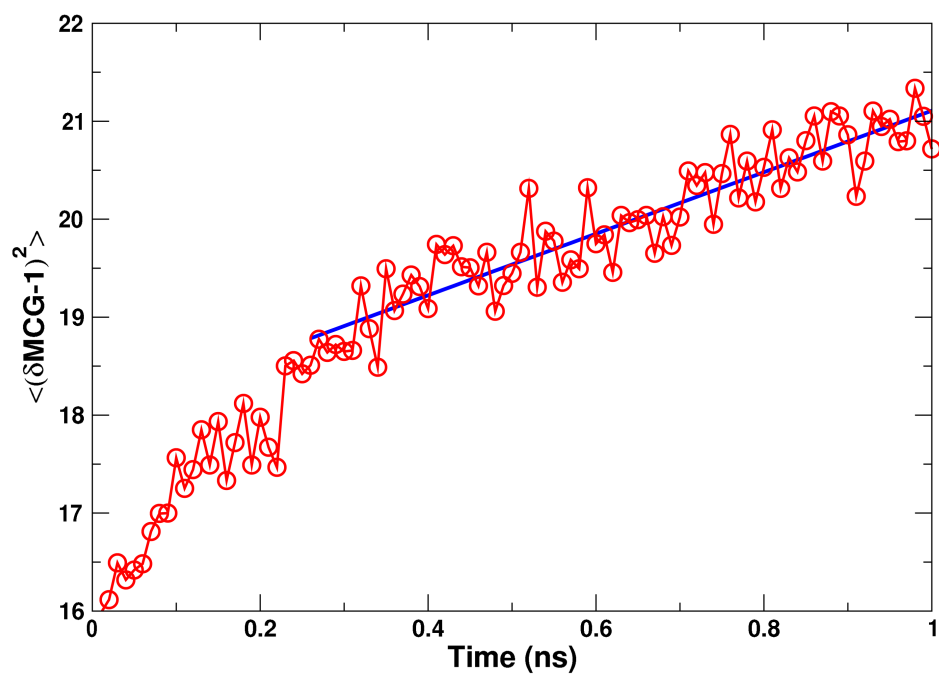


Figure S2: Diffusivity along the MCG-1 reaction coordinate. Analysis was performed on the initial 1 ns of MD trajectories from the p_B histogram test. Linear regression after initial 250 ps transient is shown in blue.