

Abstract Submitted  
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**Study of methane hydrate nucleation by accelerated molecular simulation**<sup>1</sup> YUANFEI BI, TIANSHU LI, the George Washington University — Recently clathrate hydrates have gained increasing attention due to their significance in energy, environment, safety, and gas transportation. The formation of such important compounds remains elusive, as a molecular level understanding of the nucleation mechanism is still missing. To gain such understanding, we combined forward flux sampling method with molecular dynamics, to simulate the nucleation process of methane hydrate. In particular, we have developed an effective order parameter that allows calculating hydrate nucleation rate explicitly for the first time. The order parameter is constructed based on the topological analysis of the tetrahedral network, and is capable of efficiently distinguishing hydrate from ice and liquid water. Employing this approach, we conducted molecular simulation under different thermodynamics conditions. Ensembles of nucleation pathways, containing both crystalline and amorphous hydrate nuclei, were obtained and analyzed under different conditions. In particular, pressure was found to significantly affect hydrate nucleation rate and pathways.

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