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A new method for studying nucleation in aqueous environment[1]
RAFFAELA CABRIOLU, TIANSHU LI, Department of Civil and Environmental Engineering, George Washington University — Probing nucleation of crystals in aqueous environment at the molecular level poses a major challenge in molecular simulations. The challenges are primarily attributed to two types of slow dynamics ubiquitously present in the nucleation process in aqueous environment: the rare event nature of nucleation and the sluggish dynamics of hydrogen-bond network. While advanced sampling method, such as transition path sampling or forward flux sampling, allows surpassing free energy barrier efficiently, it is unlikely to alleviate the second type of slow dynamics. Here we propose a new approach that combines Monte Carlo and molecular dynamics methods, to overcome the slow natural dynamics of tetrahedral bond network. The new approach exploits the flexibility of Monte Carlo trial moves and the collective motion of molecular dynamics. Recognizing the structural similarities between silicon and water (both belonging to "tetrahedral materials"), we incorporate the bond-switching Monte Carlo move that was developed for generating random-network models for amorphous silicon, into our approach. The approach will allow modeling nucleation of ice or hydrates based on full atomistic water model.

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