Abstract Submitted
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Computational studies of the 2D self-assembly of bacterial microcompartment shell proteins[1] JYOTI MAHALIK, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, KIRSTEN BROWN, Chemistry Department, Mercer University, XIAOLIN CHENG, UT/ORNL Center for Molecular Biophysics, MIGUEL FUENTES-CABRERA, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Bacterial microcomartments (BMCs) are subcellular organelles that exist within wide variety of bacteria and function like nano-reactors. Among the different types of BMCs known, the carboxysome has been studied the most. The carboxysomes plays an important role in the transport of metabolites across its outer proteinaceous shell. Plenty of studies have investigated the structure of this shell, yet little is known about its self-assembly . Understanding the self-assembly process of BMCs' shell might allow disrupting their functioning and designing new synthetic nano-reactors. We have investigated the self-assembly process of a major protein component of the carboxysome's shell using a Monte Carlo technique that employed a coarse-grained protein model that was calibrated with the all-atomistic potential of mean force. The simulations reveal that this protein self-assembles into clusters that resemble what were seen experimentally in 2D layers. Further analysis of the simulation results suggests that the 2D self-assembly of carboxysome's facets is driven by nucleation-growth process, which in turn could play an important role in the hierarchical self-assembly of BMCs' shell in general.

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