Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Simulations of polymorphic icosahedral shells assembling around many cargo molecules[1] FARZANEH MOHAJERANI, JASON PERLMUTTER, MICHAEL HAGAN, Brandeis University — Bacterial microcompartments (BMCs) are large icosahedral shells that sequester the enzymes and reactants responsible for particular metabolic pathways in bacteria. Although different BMCs vary in size and encapsulate different cargoes, they are constructed from similar pentameric and hexameric shell proteins. Despite recent groundbreaking experiments which visualized the formation of individual BMCs, the detailed assembly pathways and the factors which control shell size remain unclear. In this talk, we describe theoretical and computational models that describe the dynamical encapsulation of hundreds of cargo molecules by self-assembling icosahedral shells. We present phase diagrams and analysis of dynamical simulation trajectories showing how the thermodynamics, assembly pathways, and emergent structures depend on the interactions among shell proteins and cargo molecules. Our model suggests a mechanism for controlling insertion of the 12 pentamers required for a closed shell topology, and the relationship between assembly pathway and BMC size polydispersity. In addition to elucidating how native BMCs assemble,our results establish principles for reengineering BMCs or viral capsids as customizable nanoreactors that can assemble around a programmable set of enzymes and reactants.

[1]Supported by NIH R01GM108021 and Brandeis MRSEC DMR-1420382.

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Date submitted: 10 Nov 2016 Electronic form version 1.4