Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Atomistic simulations of the MS2 coat protein conformational transition MATTHEW PERKETT, FRANCESCO PONTIGGIA, MICHAEL HAGAN, Brandeis University — During the replication of many viruses, hundreds to thousands of proteins self-assemble to form a protective protein coat, called a capsid, around the viral nucleic acid. Often these proteins have identical amino acid sequences with slightly different, or quasi-equivalent, conformations, which join in precise spatial arrangements. Although the structure of completed capsids is known to atomic resolution, little is known about the assembly intermediates and how protein conformations are selected during assembly. In this talk, we will use all-atom simulations to investigate how protein-RNA interactions guide conformational transitions of capsid proteins from the single-stranded RNA bacteriophage MS2. Since conformational changes occur on timescales which are not accessible to all-atom simulations, we use enhanced sampling methods to sample probable transition pathways and corresponding free energy profiles. Specifically, we will present free energy profiles associated with the MS2 capsid protein conformation in the presence and absence of RNA.

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Date submitted: 11 Nov 2011 Electronic form version 1.4