

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Modeling the Crystallization of Proteins HONGJUN LIU, SANAT KUMAR, Columbia University, SHEKHAR GARDE, RPI — We have used molecular dynamics and monte carlo simulations to understand the pathway to protein crystallization. We find that models which ignore the patchy nature of protein-protein interactions only crystallize inside the metastable gas-liquid coexistence region. In this regime they crystallize through the formation of a critical nucleus. In contrast, when patchiness is introduced we find that there is no need to be inside this metastable gas-liquid boundary. Rather, crystallization occurs through an intermediate which is composed of disordered aggregates. These are formed by patchy interactions. Further, there appears to be no need for the formation of a critical nucleus. Thus the pathways for crystallization are strongly controlled by the nature of protein-protein interactions, in good agreement with current experiments.

Hongjun Liu
Columbia University

Date submitted: 20 Nov 2006

Electronic form version 1.4