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Water dynamics during the association of hiv capsid proteins studied by all-atom simulations[1] NAIYIN YU, MICHAEL HAGAN, Brandeis University — The C-terminal domain of the HIV-1 capsid protein (CA-C) plays an important role in the assembly of the mature capsid. We have used molecular dynamics simulations combined with enhanced sampling methods to study the association of two CA-C proteins in atomistic detail. In this talk we will discuss the dynamics of water during the association process. In particular, we will show that that water in the interfacial region does not undergo a liquid-vapor transition (de-wetting) during association of wild type CA-C. However, mutation of some hydrophilic residues does lead to a dewetting transition. We discuss the relationship between the arrangement of hydrophilic and hydrophobic residues and dewetting during protein association. For the HIV capsid protein, the arrangement of hydrophilic residues contributes to maintaining weak interactions, which are crucial for successful assembly.

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