Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Exploring the dewetting transition in the hydrophobic collapse of melittin PATRICK VARILLY, University of California, Berkeley, AMISH J. PATEL, Rensselaer Polytechnic Institute, DAVID CHANDLER, University of California, Berkeley — We present our recent results on understanding the hydrophobic collapse of melittin dimers. Melittin dimers have large, complementary hydrophobic patches, and the dimer collapse mechanism involves a dewetting transition [Liu, Huang, Zhou and Berne, *Nature* **437**, 159–162 (2005)]. As a result, melittin has become a model system for studying dewetting transitions in proteins. We apply our recently- developed tools for probing density fluctuations in water [Patel, Varilly and Chandler, *JPCB* **114**, 1632–1637 (2010)] to understand this dewetting transition in terms of free energy surfaces, their bistability and their barrier heights. We show how the hydrophobic character of melittin's tetramerization surface results in an enhanced probability of density depletion next to that surface. When two dimers come together, the density depletion is further enhanced, so that even at large separations, there is a metastable dry phase in the region between the dimers. As the dimers come together, the dry phase is stabilized and eventually the wet phase is destabilized, leading to the collapse of the dimers. We explore how mutations that have been observed to suppress the dewetting transition affect the corresponding free energy surfaces and discuss our ongoing efforts to fully map out the reaction coordinate of melittin collapse.

Patrick Varilly
University of California, Berkeley

Date submitted: 19 Nov 2010

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