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Pack and split: a simulation study of structural transitions of sodium dodecyl sulfate micelles MARIA SAMMALKORPI, Yale University, MIKKO KARTTUNEN, University of Western Ontario, MIKKO HAATAJA, Princeton University — Surfactants are important interfacial agents in many biological and industrial systems. Their self-assembly and versatility of the aggregates lies at the heart of all biological membrane, vesicle and micelle formation, and many industrial solubilization processes. While biologically and industrially extremely important, surprisingly little is known about molecular details of the self-assembly of surfactants and the dynamics of the formed structures. Here we extend our previous work of model construction and structural properties of self-assembled sodium dodecyl sulfate (SDS) micelles [J. Phys. Chem. B 111, 11722 (2007)] to structural transitions of these self-aggregates. We present the results of detailed molecular dynamics simulations of anionic micelle fission, and structural changes in the micelles brought forth by differences in the ionic strength of the solution [J. Phys. Chem. B 113, 5863 (2009);J. Am. Chem. Soc. 130, 17977 (2008)]. We demonstrate the existence of a new fission pathway which consists of a Rayleigh instability driven by Coulombic interactions, and a formation of a long interdigitating stalk.

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