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Self-assembly of ionic detergents: a simulation study of sodium dodecyl sulfate micellization MARIA SAMMALKORPI, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA, MIKKO KARTTUNEN, Department of Applied Mathematics, University of Western Ontario, Middlesex College, 1151 Richmond St. North, London (ON), Canada, MIKKO HAATAJA, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA — Detergents, amphiphilic molecules used to separate and dissolve molecular aggregates and also as cleaning agents, consist of a polar head group and one or more hydrophobic tails. Above a critical concentration, they self-aggregate in an aqueous solution to form micelles. While industrially extremely important, surprisingly little is known about molecular details of the self-assembly of detergents. Here we extend our previous work of modeling and model construction of charged soft-matter systems [1] by a description of an anionic detergent, sodium dodecyl sulfate (SDS) [2]. We present the results of large-scale Molecular Dynamics simulations of the formation dynamics and structure of SDS micelles. We demonstrate that temperature affects micelle morphologies through the packing and discuss the effect of SDS concentration on the micellization.
[1] M. Patra et al., Biophys. J. 84, 3636 (2003); A. A. Gurtovenko et al., J. Phys. Chem. B 109, 21126 (2005); A. A. Gurtovenko et al., Biophys. J. 86, 3461 (2004).
[2] The SDS parameters are available at www.softsimu.org.

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