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Breaking it up: Simulations of micelle fission in explicit solvent MIKKO KARTTUNEN, The University of Western Ontario, MARIA SAMMALKORPI, MIKKO HAATAJA, Princeton University — We study self-assembly in micellar systems consisting of sodium dodecyl sulfate (SDS) using detailed 200-400 ns atomic scale molecular dynamics simulations. The simulations were done with explicit solvent, counterions and salt. We focus on the role of molecular level interactions driving self-assembly [1] and, in particular, show how micelle fission can be controlled using electrostatics. As our main result, we demonstrate the existence of a new fission pathway in charged micelles [2] and provide a physical explanation for it.

1. M. Sammalkorpi, M. Karttunen, M. Haataja, J. Phys. Chem. B **111**, 11722 (2007).
2. M. Sammalkorpi, M. Karttunen, M. Haataja, J. Am. Chem. Soc., in press.

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