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The effect of block-copolymer structures on the polymeric liquid-liquid interface: Molecular Dynamic Study JIHO RYU, WON BO LEE[1], Sogang Univ, BUMJOON KIM[2], KAIST — The change of free energy caused by different morphology of surfactants (block- and grafted-copolymers) in the biphasic system, is investigated by molecular dynamic simulations. We studied two different structures of surfactants. Type 1 is a diblock-copolymer surfactant composed with 60 monomers(30 A beads and 30 B beads). Type 2 is a grafted-copolymer surfactant of which two side chains composed of, respectively, 15 B monomers, are attached to main back bone chain composed of 30 A monomers. All simulations were performed in the NVT ensemble at 373K. Free energy are computed by thermodynamic integration from the coupled state to the uncoupled state where the surfactant does not interact with the biphasic system. In addition, we discuss various effects such as stiffness of polymers.

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