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连接基团与尾链长度对阳离子Gemini表面活性剂与阴离子聚电解质复合物影响的分子动力学模拟

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摘要 Interaction of anionic polyelectrolyte with cationic gemini surfactant has been investigated by coarse-grained molecular dynamics simulation. Polyelectrolyte facilitates the oppositely charged ionic surfactants to aggregate by suppressing the electrostatic repulsion between ionic head groups leading to the formation of micellar complex. With addition of surfactant, the conformation of polyion chain changes from stretched to random coiled to spherical, and at the same time more free micelles are formed by surfactants in mixtures. Increasing the length of spacer or tail chain in gemini surfactant will weaken its interaction with polyelectrolyte and simultaneously strengthen its tendency to self-assemble. The simulation results are consistent with experimental observations and reveal that the electrostatic interaction plays an important role in the interaction of polyelectrolyte with gemini sur-factant.

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Molecular dynamics simulation for the effect of chain length of spacer and tail of cationic gemini surfactant on the complex with anionic polyelectrolyte

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Key words interaction; polyelectrolyte; gemini surfactant; molecular dynamics

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