# Study on Adsorption Behavior of a New Type Gemini Surfactant onto Quartz Surface by Molecular Dynamics Method

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**Abstract.** Compared with traditional single-chain surfactants, Gemini surfactants have lower critical micelle concentration (CMC) and higher surface activity. The adsorption mechanism of the branched quaternary ammonium salt Gemini surfactant (Gemini C3) at the water-surfactant-quartz interfaces is studied by Molecular Dynamics (MD) method. Simulation snapshots of the Gemini C3 adsorption configuration show the molecules in the first layer are adsorbed with all the head groups facing the neutral quartz surface, and those in the second layer move into the water layer forming micelles by self-assembly. The relative concentration profile is higher in the first layer. Mean square displacement (MSD) curve of surfactant molecules gradually increases in the range from 150 to 500 ps, and become significantly larger than that of the water molecules after 250 ps. for the moving of surfactant molecules and the separation of two layers. More water molecules around the head group of the surfactant molecules are observed after the response to imply the formation of aggregated structure with increasing interaction between them. This work revealed the microscopic adsorption mechanism of the Gemini C3 surfactant onto the quartz surface, and provided theoretical guidance for controlling the wetting properties and surface modification of the rock, highlighting the potential for EOR.