Molecular Dynamics Simulation of Adsorption Behavior of Schiff base Gemini Surfactants on Zn (1 1 0) Surface

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Molecular dynamics simulation method was selected to investigate the adsorption behavior of three quaternary ammonium Schiff base Gemini surfactants on Zn (1 1 0) surface, including 4,4'-(hydrazine-1,2-diylidenebis-(methanylylidene))bis-(N-decyl-N,N-dimethylbenzenaminium)bromide(D1), 4,4'-(hydrazine-1,2-diylidenebis(methanylylidene))bis(N-dodecyl-N,N-dimethylbenzenaminium) bromide (D2), and 4,4'-(hydrazine-1,2-diylidenebis(methanylylidene))bis(N-myristyl-N,N-dimethylbenzenaminium)bromide(D3). The electrochemical impedance spectroscopy (EIS) and scanning electron microscope (SEM) showed that D3 had better corrosion inhibition performance for the zinc electrode and more excellent inhibitory effect on dendrite, deformation and passivation of zinc. The molecular dynamics simulation results indicated that the order of adsorption energy of three Schiff base Gemini surfactants was D3>D2>D1, the adsorption rate followed the order of D3 >D2 > D1. The adsorption energy was greater and the adsorption rate was faster, D3 had the best effect on corrosion inhibition, inhibiting dendrite and deformation.

Keywords: Schiff base Gemini surfactants; molecular dynamics simulation; adsorption behavior; corrosion inhibition

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