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**Molecular dynamics simulation of methane hydrate formation
on metal surface with oil**

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ABSTRACT

Microsecond molecular dynamics simulations were performed to investigate the methane hydrate formation on smooth and rough metal surface covered with water, light oil, and heavy oil with asphaltenes, respectively. The growth and crystallization of methane hydrates were characterized by the four-body order parameter and the face-saturated incomplete cage analysis. Results highlighted the priority for hydrate growth inside the groove of rough metal surface, from which the hydrate grew upwards to the outside of the groove and then to the water-gas interface. It clearly

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