Study of the physical chemistry properties of asphaltene-aggregation process by Molecular Dynamics.

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Asphaltenes are the main component of the heavy-weight fraction of crude oil, and they can be described as a family of molecules with at least one aromatic carbon nuclei, in which both heteroatoms and alkylic side chains can also be present. Due to their physical chemistry properties, asphaltenes tend to aggregate themselves and precipitate, which can cause several problems throughout the refining operations, such as the clogging of pipelines. However, aggregation is a series of complex processes that are triggered by numerous factors, namely temperature, pressure, and even the composition of the oil mixture. Therefore, not only has there been a growing interest to understand this aggregation phenomenon, but also to develop alternatives to prevent it.

Nowadays, classical molecular dynamics simulations are capable of fully describing the behavior of many complex aggregation systems, including asphaltenes. These methods allow the implementation of strategies to obtain successive configurations of any evolving system and calculate certain properties, such as free energy and kinetics measures that can be compared with experimental data.