

Abstract Submitted
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Mesoscale simulation of asphaltene aggregation¹ JIANG WANG, ANDREW FERGUSON, University of Illinois Urbana-Champaign — Asphaltenes constitute a heavy aromatic crude oil fraction that can aggregate and precipitate out of solution. Association is thought to proceed hierarchically according to the Yen-Mullins model, but the molecular mechanisms and pathways remain poorly understood. In this study, we perform molecular dynamics simulations of the aggregation of hundreds of asphaltenes over microseconds using the coarse-grained Martini force field. We identified a hierarchical self-assembly mechanism consistent with Yen-Mullins model, but the details of which are strongly dependent on asphaltene molecular structure. Monomeric asphaltenes first self-assemble into 1-D rod-like nanoaggregates, followed by the formation of clusters of nanoaggregates. At high concentrations, asphaltenes with short aliphatic side chains assemble into a percolating network with the binding of 1-D rods. Conversely, molecules with more and longer side chains cannot efficiently stack, producing a fractal network of 1-D rods suspended in a sea of interpenetrating aliphatic side chains. Our results provide the first molecularly-detailed validation of the full Yen-Mullins hierarchy, and are in good agreement with recent computational and experimental studies.

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