Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

New insight into the role of the self-assembly of heteroatom compounds in heavy oil viscosity enhancement

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In this simulation, a total of eight alkanes were employed to represent the various components of heavy crude oil. These alkanes included hexane, heptane, octane, nonane, cycloheptane, cyclohexane, benzene, and toluene (Fig. S1).

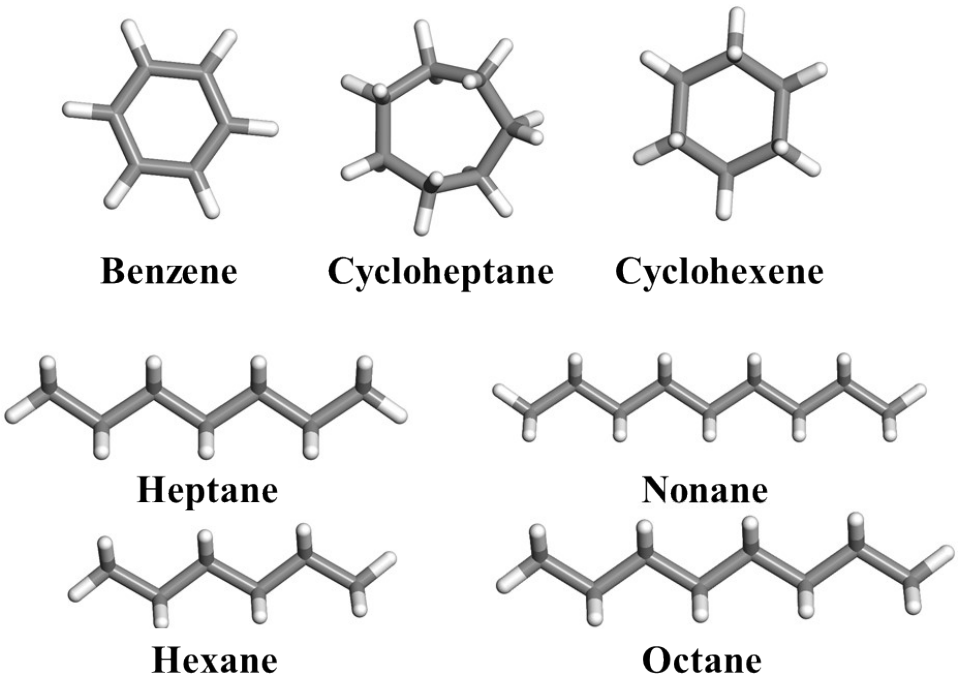

Fig. S1. The molecular structure of light oil components.

Non-covalent interaction (NCI) analysis is widely used to visually represent the location and characteristics of non-covalent interactions between molecules. This method utilizes the reduced density gradient (RDG) isosurface to depict regions of non-covalent interactions. By colorfully mapping the (λ2)ρ function onto the RDG isosurface, the nature of intermolecular interactions can be effectively illustrated (Fig. S3).

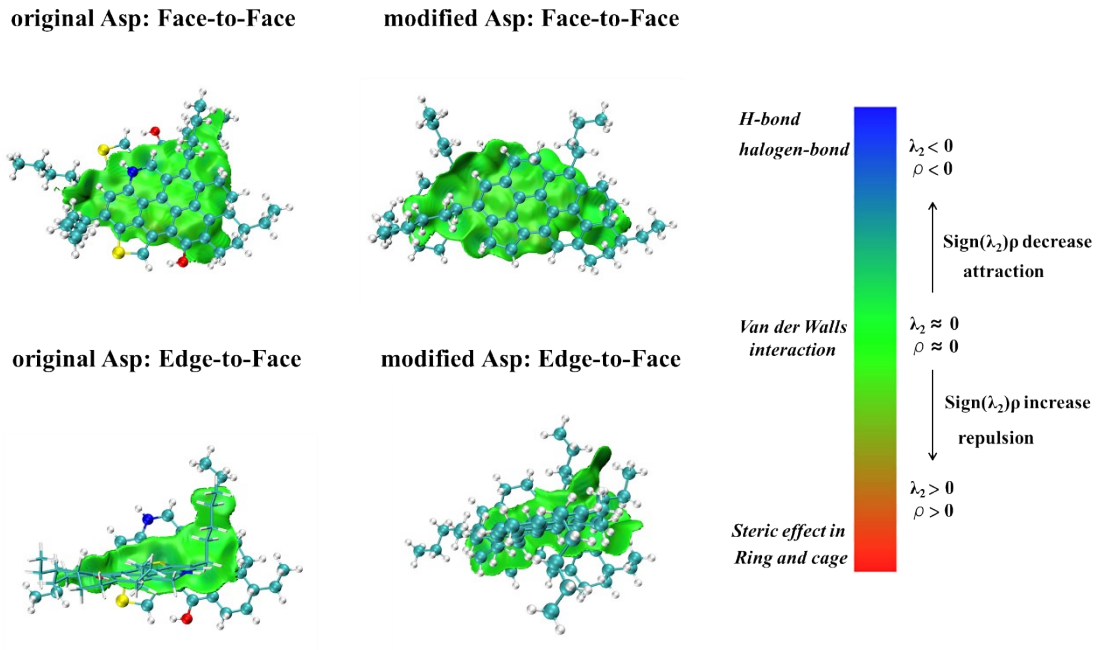

Fig. S2. Optimized structures and NCI maps of asphaltene dimers.

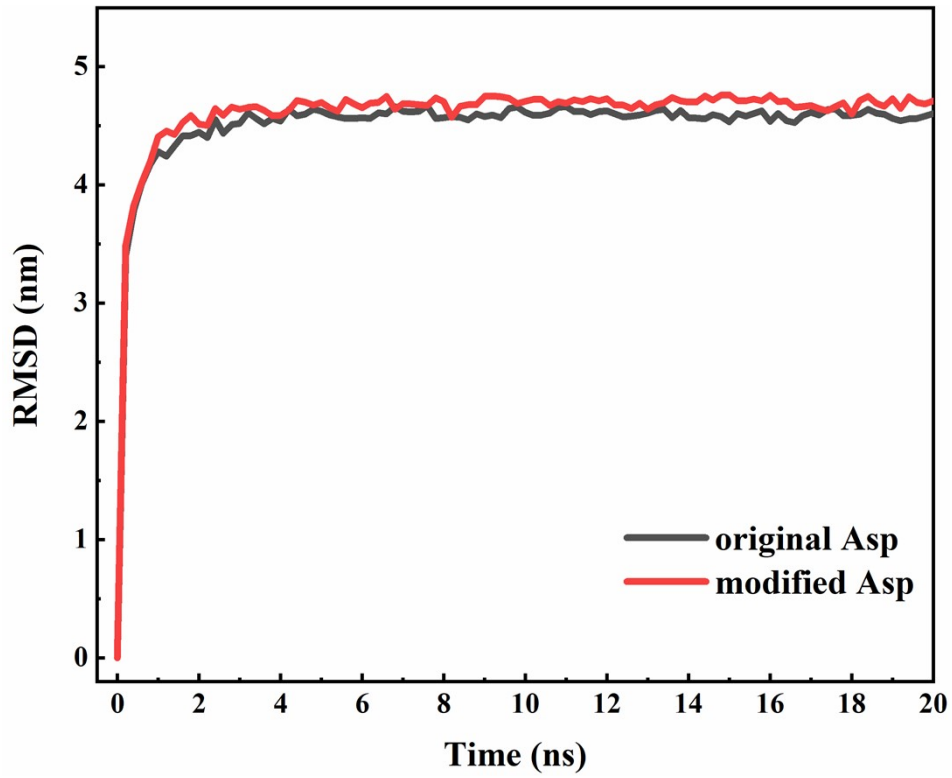

Fig. S3. The root-mean-square-displacement for the two studied systems.

The value of Coordination number (CN) has been computed at the positions of minima after and before the peak, according to your suggestion as shown in Fig. S4. From the Fig. S4, it can be observed that the face-to-face stacking structure of asphaltene molecules exhibits a higher CN value compared to the edge-to-face stacking structure.

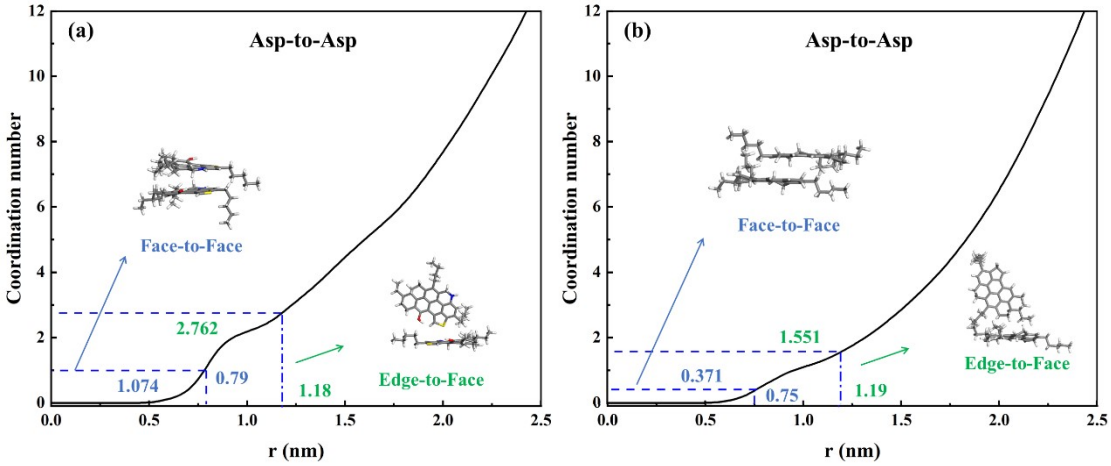

Fig. S4. Coordination number between asphaltene molecules in (a) original Asp system and (b) modified Asp system.

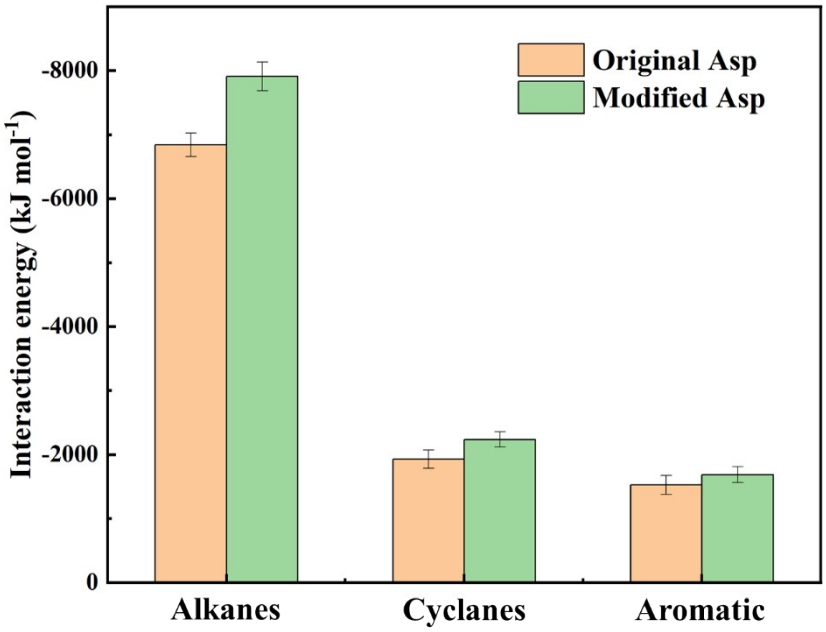

Fig. S5. Interaction energy between asphaltenes and hydrocarbon during last 2 ns.