Atomistic modelling of oil shale kerogen and asphaltene

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Atomistic modeling is routinely used in many industries (pharmaceutical, polymers, coatings, explosives, membrane proteins, etc.) to gain insight into the properties of materials. In the case of petroleum precursors, *e.g.*, source rocks, asphaltene, and kerogen, little information is presently available to describe the physical behavior of and/or their interaction with mineral matrices. Here Siskin's two-dimensional structures of the kerogen and asphaltene were used as starting points to develop three-dimensional models. Preliminary chemical structures were obtained via the molecular mechanics energy minimization using force fields. These minimized structures were further optimized using *ab initio* methods. These monomer structures were further used to explore the importance of stacking and aggregation on spectroscopic properties of these compounds. Using the three dimensional molecular models it was possible to calculate molecular properties that can be correlated with experimental data obtained from solid and liquid state ^{13}C NMR spectroscopy, atomic pair-wise distribution functions, TGA data on pyrolysis kinetics, small angle X-ray scattering, and ICR-mass spectroscopy. The calculated properties are quite sensitive to the three dimensional models and the underlying two models used in their construction. The calculated properties show overall agreement with their respective measurements, but the agreement is not exact. The lack of agreement may be due to deficiencies in our models and/or to the inherent inhomogeneity of natural samples. This issue is currently under investigation. Our work shows that molecular modeling is a viable technique to provide atomistic scale representation of the structure and environment of oil shale kerogen and oil sand asphaltene. Molecular properties calculated with these models present sensitivity to these models, indicating that they can be used to guide further model refinements. Finally, verified models can be used to test new processing approaches for exploitation of these resources.