Molecular Simulations of Organic Semiconductors for Clean Energy Production

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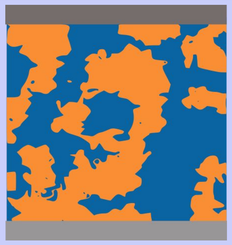
1. Introduction



Controlling the spontaneous aggregation of conjugated molecules provides opportunities to engineer the next generation of photovoltaic devices and prevent oil pipe blockage. In organic photovoltaics, aggregation is beneficial for blends of electron donating/accepting compounds (left) which control and allow for the generation of electricity from light. In oil extraction, aggregation of conjugated molecules called asphaltenes (right) caused by changes in pressure and solvent is detrimental and expensive to remove. By understanding the structure and spontaneous aggregation of conjugated molecules we can simultaneously improve energy production by furthering the next generation of clean, renewable energy and increase the efficiency of current oil extraction methods.

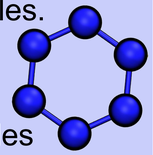
2. Development

Our simulations are run using HOOMD-Blue. The molecular building blocks were constructed with mBuild.

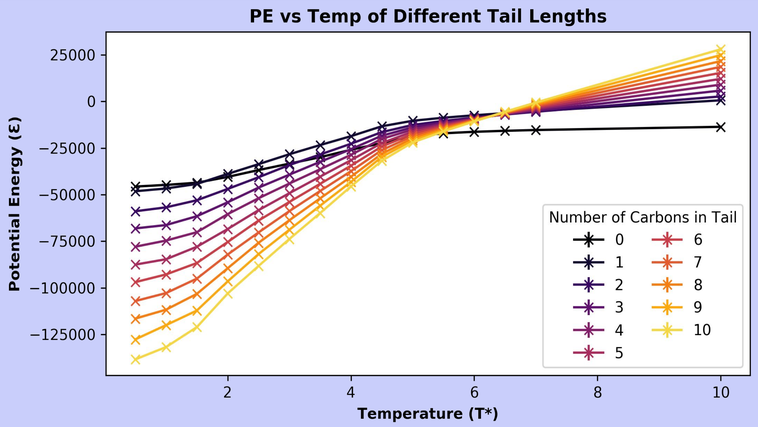
To minimize the computational expense of the simulations we utilize the United Atom model, which includes hydrogens implicitly in its potentials

Aromatic rings are modeled as rigid bodies for additional speed improvements. We develop code for testing assemblies of polyaromatic molecules.

Molecules of increasing complexity are studied, beginning with rigid benzene, then benzenes with tails, and polyaromatic molecules



4. Analysis

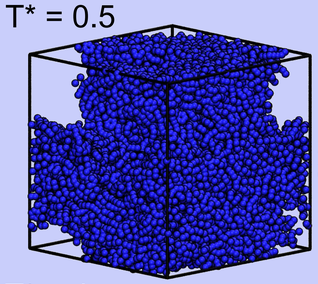


Above is a graph of the evolution of potential energy as a function of temperature for simulations containing benzene with one tail. This point is virtually the same for all benzene with tails. It can be observed that as the chain length increases, the potential energy at the point of order to disorder decreases.

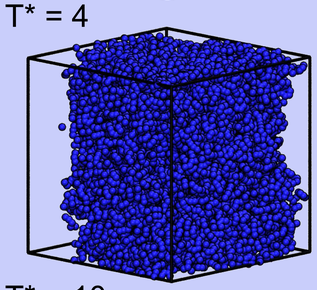
The simulations were interpreted using Visual Molecular Dynamics (VMD), which helped show the point of order to disorder. Analysis also consisted of observing the Radial Distribution Functions of the simulations, which helped determine the state of the molecules.

3. Molecular Dynamics

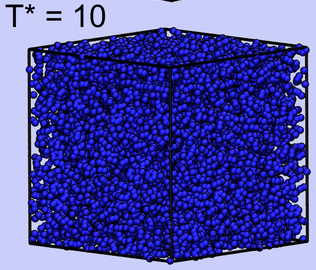
T* = 0.5



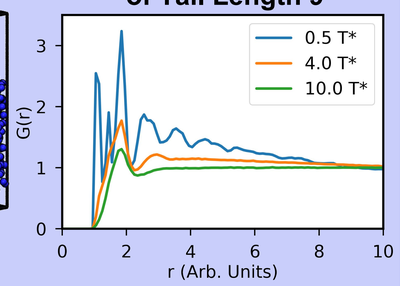
T* = 4



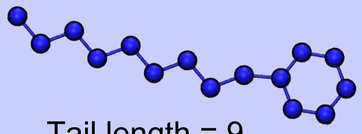
T* = 10



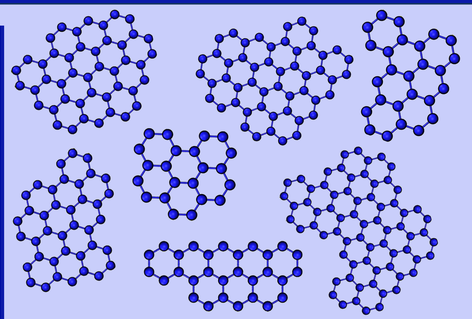
Different Temperatures of Tail Length 9



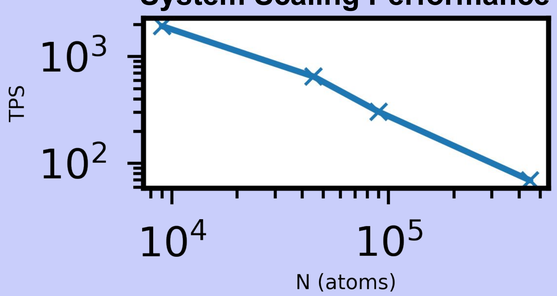
Systems of benzenes with with tail lengths from 1 - 10 carbons were equilibrated. The simulations were run for 1e6 timesteps (ranged from 10-40 min). The lowest temperatures were run for 2e7 timesteps to verify equilibration (about 2hrs).



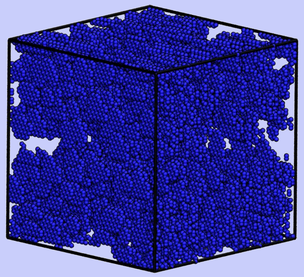
Tail length = 9



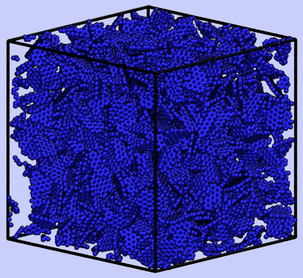
System Scaling Performance



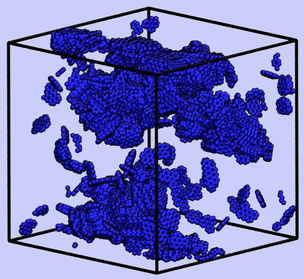
To simulate simplified asphaltenes we automate the generation of random polyaromatic cores (above). Pictured below are snapshots of polydisperse asphaltenes with that have been cooled from high to low temperature. The time taken to initialize molecules containing more than 50,000 molecules increased significantly (~12 hrs), and equilibration was not observed until at least 200 million timesteps had passed. The largest system sizes that we ran here are 450,000 atoms.



Initial configuration



T* = 7



T* = 1

5. Conclusion and Outlook

In this work, we are able to initialize large systems of diverse molecules and reach equilibration within a day enabling analysis into what state the molecules are in and what properties the molecules might have, including the vaporization of benzene with and without different aliphatic chains. Additionally, we demonstrated the aggregation of asphaltenes through annealing simulations, were able to simulate large systems of benzene, control the length of the side chains, and began the development of a script to generate large polyaromatic hydrocarbons. Future research will work to expand our initialization scripts in order to investigate assemblies of polydisperse asphaltenes in both organic photovoltaics and oil extraction applications.

6. Acknowledgements

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Goual, L. *Petroleum Asphaltenes* **2** (2012)