

Supplemental Information : Understanding the nanoscale structure of hexagonal phase lyotropic liquid crystal membranes

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TODO : These are things I am working on / need to do

- Initial configuration dependence
 - Initial pore-to-pore spacing
 - Initial pore radius
 - I have simulations running to support the claims that these are not significant factors if chosen within reason
- Description of parameterization process
- Feel free to suggest anything else that might be useful

Calculation of pore-to-pore spacing statistics

This is an outline of this section and will be reworded for clarity

- We are interested in 5 pore-to-pore distances which should all be equal in a perfect hexagonal array, however only 4 distances are independent visualize this in supplemental material. Will make a lot of things more clear below.
- Each pore spacing has its own trajectory of spacing vs. time. Using data collected after the system is equilibrated, we calculate how long it takes for the data in each of the 5 trajectories to become uncorrelated using `pymbar.timeseries.integratedAutocorrelationTime()`
- We break the full trajectories down into sub-trajectories based on the maximum autocorrelation time of those found in the previous step.
- For each bootstrap trial, we recreate an equilibrium trajectory by randomly sampling pore spacings from the sub-trajectories
- We get an average value for each pore spacing by finding the mean of the bootstrapped data
- We calculate the overall average as the mean of all bootstrapped pore spacings
- The uncertainty for each pore spacing is calculated as $\frac{\langle x \rangle - \bar{x}}{4}$ where $\langle x \rangle$ is the average spacing from the bootstrap trial and \bar{x} is the average value of one of the pore spacings.
- We report the mean of these uncertainties

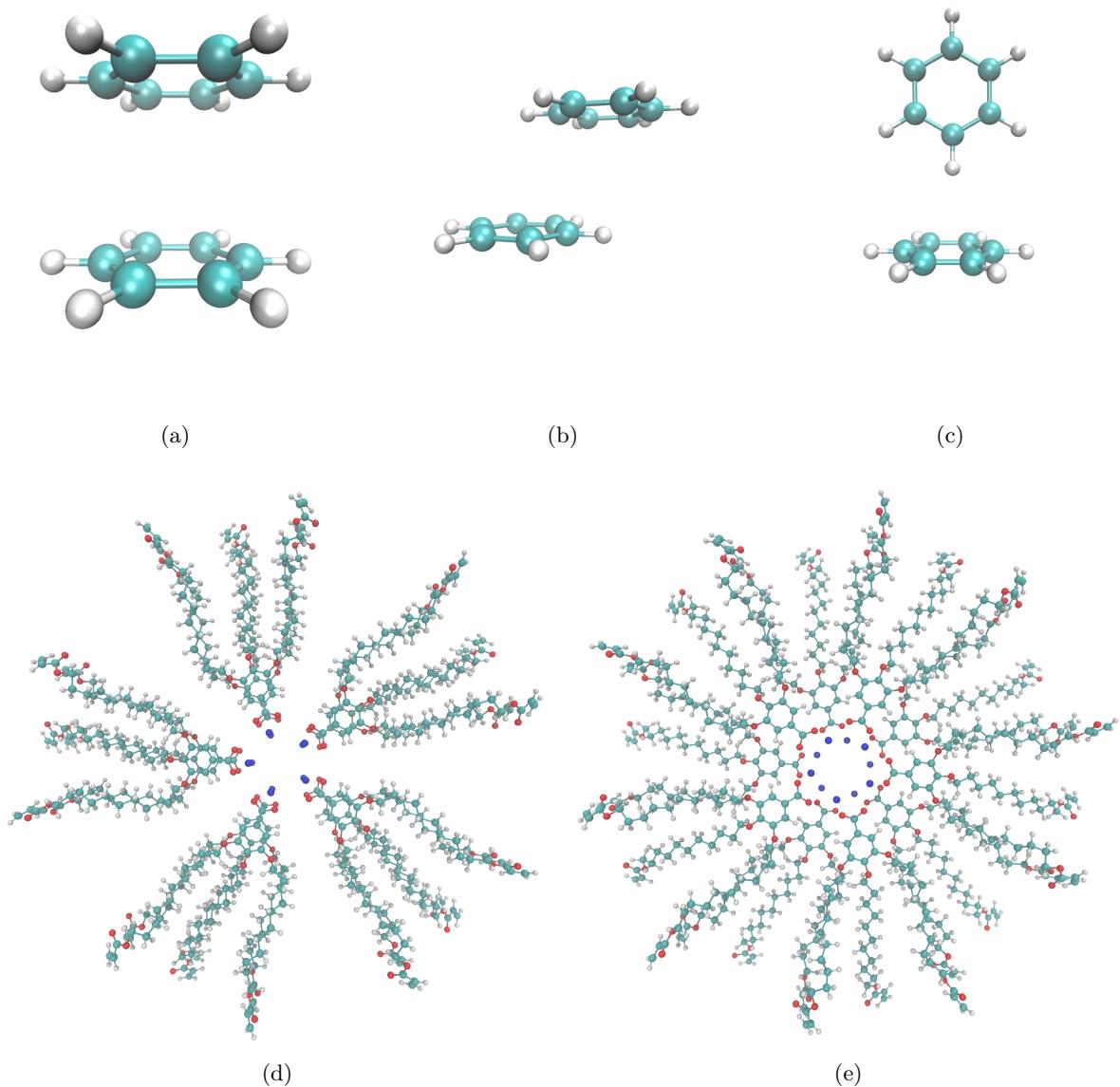


Figure 1: (a) Sandwiched benzene dimers stack 3.8 Å apart. (b) Parallel-Displaced benzene dimers stack 3.4 Å vertically and 1.6 Å horizontally apart. (c) T-shaped benzene dimers stack 5.0 Å apart. (d) Two monomer layers stacked in the sandwiched configuration (e) Two monomer layers stacked in the parallel-displaced configuration

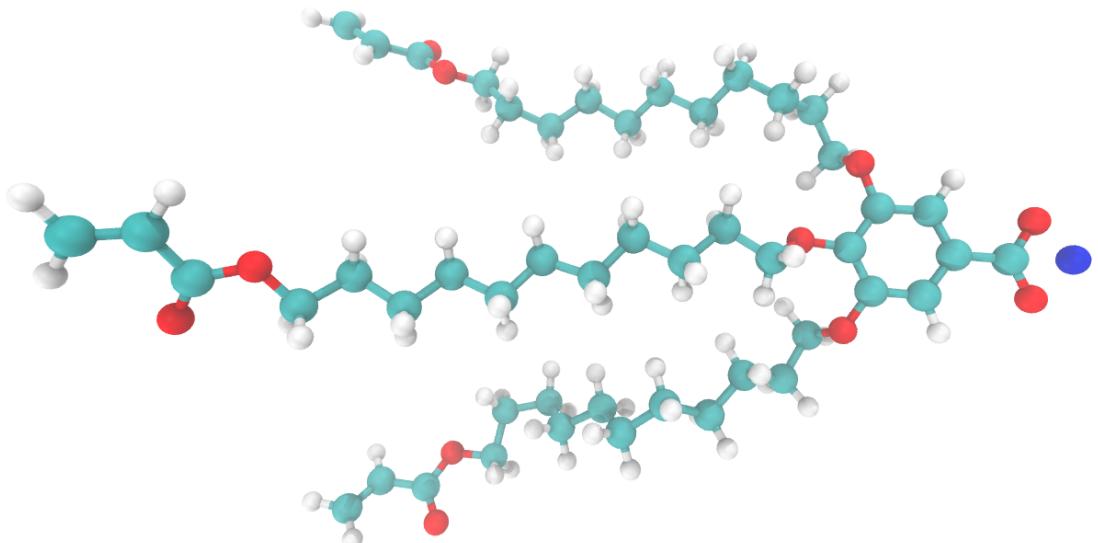


Figure 2: Atomistic representation of the monomer Na-GA3C11. White atoms represent hydrogen, cyan atoms represent carbon, red atoms represent oxygen and the blue atom is sodium.

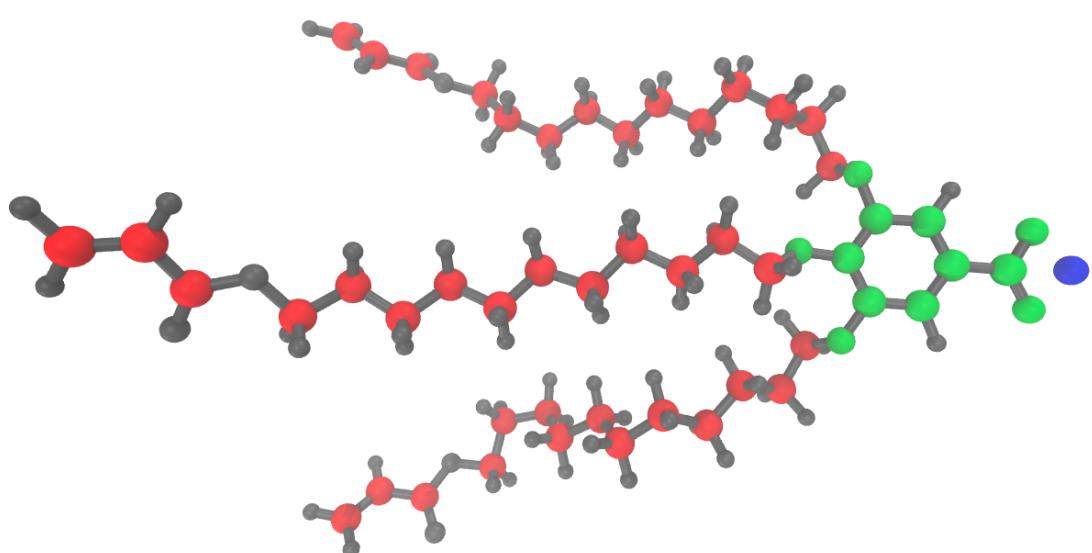


Figure 3: The groups used for $g(z)$ calculations. Red atoms are in the tails group. Green atoms are in the head group region. The blue atom is sodium.

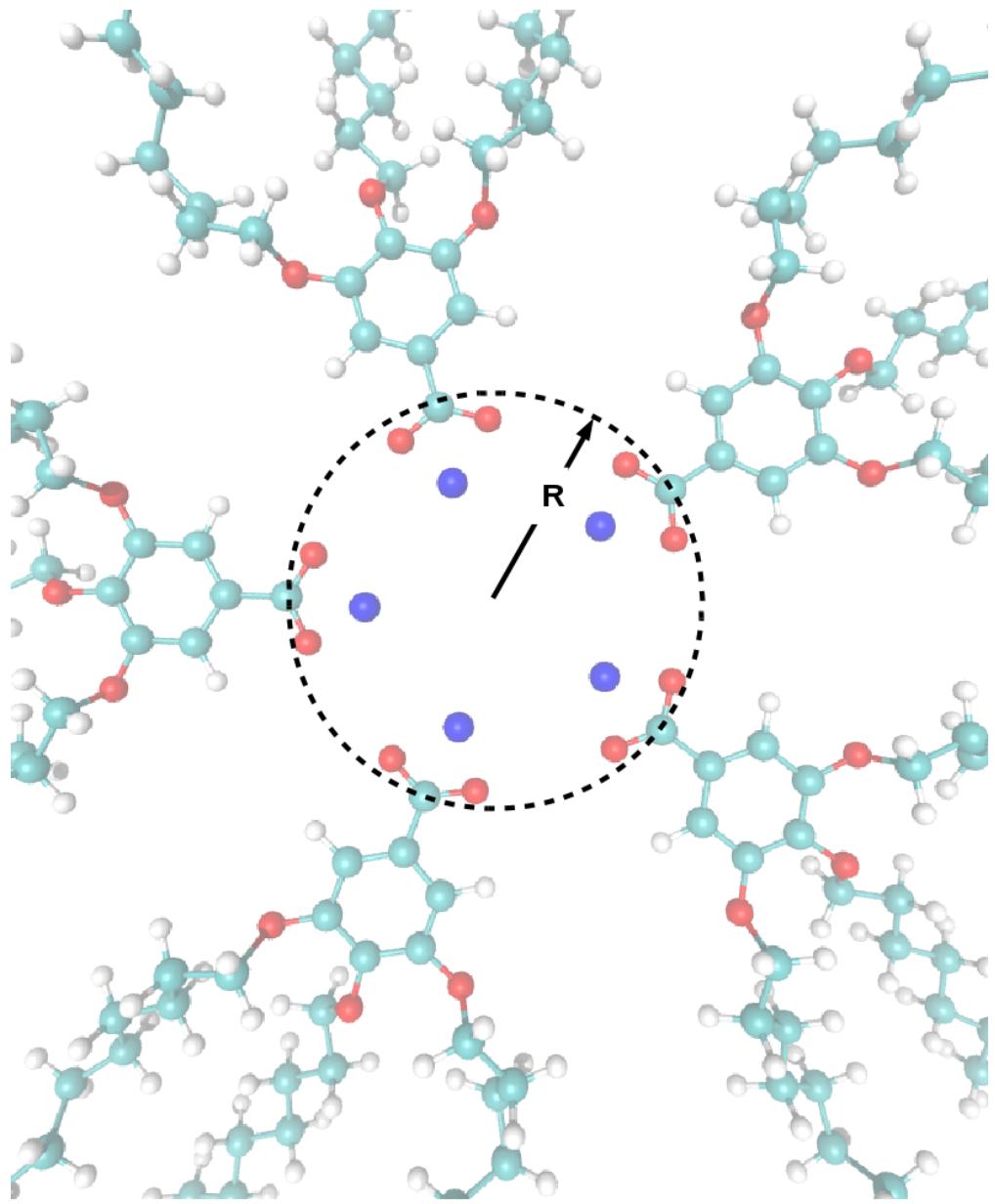


Figure 4: When creating an initial configuration, the pore radius is defined based on the distance of the carbonyl carbon from the pore's central axis

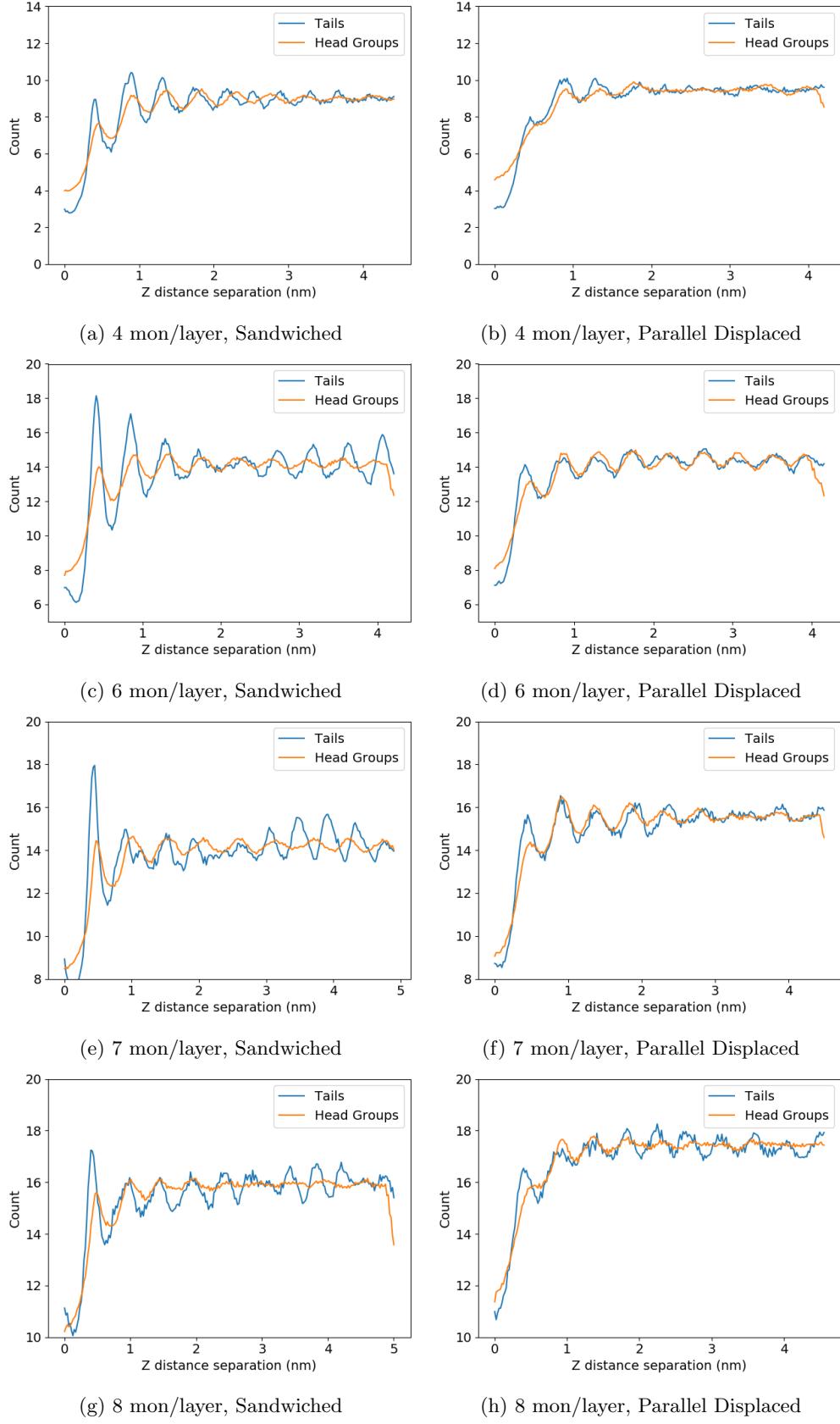


Figure 5: $g(z)$ for all other configurations built with layers stacked 3.7 Å apart

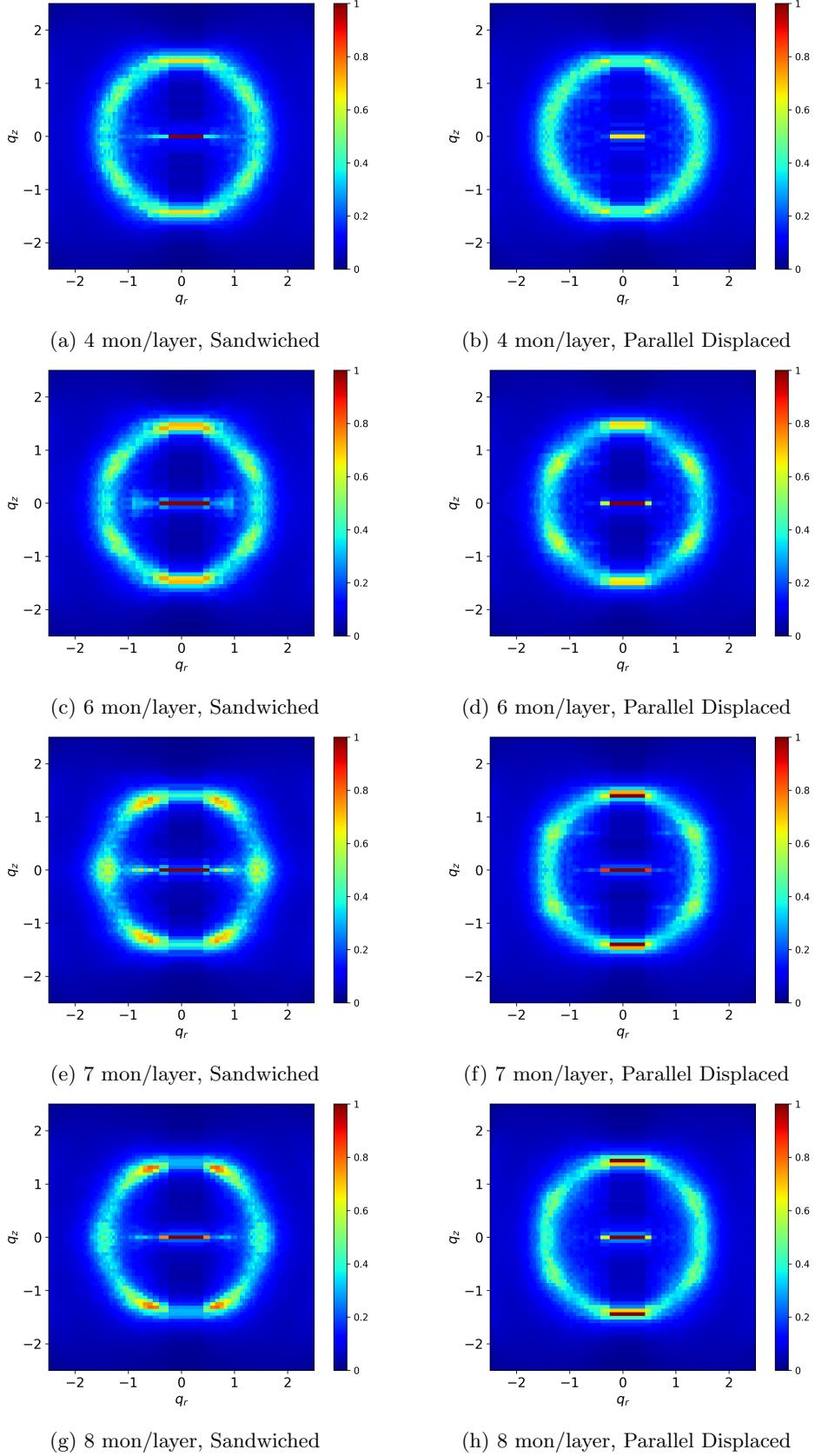


Figure 6: Simulated XRD patterns for all other configurations built with layers stacked 3.7 Å apart

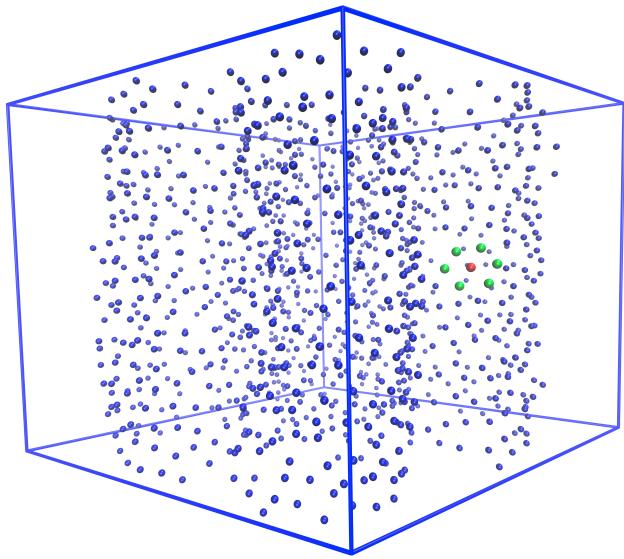


Figure 7: Monomer tails pack together hexagonally. The centroid of each tail is visualized as a blue sphere. The centroids are calculated based on the red atoms in Figure 3. The red sphere highlights an example of an alkane tail centroid with its nearest neighbors (green spheres) surrounding it in a hexagonal pattern.

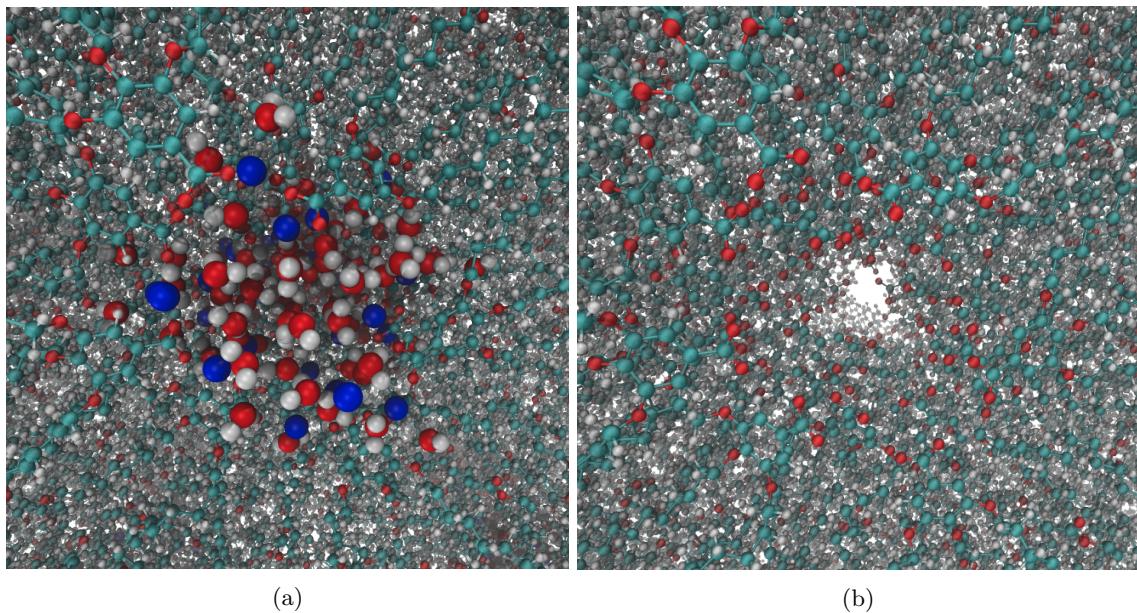


Figure 8: (a) Pores built in the parallel displaced configuration with 5 monomers per layer are filled with 5 wt% water. (b) The same system is visualized with water molecules and sodium ions removed. Head groups vacate the pore region leaving an aqueous solution of water and sodium ions.