EFFECT OF SILANE DENSITY ON WETTABILITY OF SILANE-GRAFTED SILICA

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Introduction
- Fiber-matrix adhesion is critical for transferring loads effectively and enhancing the overall strength and durability of composites.
- However, much is still left to be desired when understanding at nanoscale.
- Favorable wettability between the fiber, resin and interfacing material ensures efficient bonding in the interface region and thus load transfer.
- S-glass fibers are commonly used as reinforcement in composite materials, and their surface properties play a crucial role in determining the mechanical behavior of composites.
- Our final goal is to understand how Silane chemistries (interfacing materials), including Glycidoxypropyltrimethoxy (GPS), Aminopropyltriethoxy (APS), will affect wettability and thereby adhesion.

Why Molecular Dynamics?
It is experimentally challenging to control the variables which govern the aspects of wettability such as Bond density of silane molecule on the fiber surface, which is why MD is being utilized.

Objectives
- Realize the effect of Silane bond site density on wettability of silane-grafted silica.

Current Objectives
- Produce literature-backed Silica, Silane, Nitrogen, and Water models.
- Validation of the forcefield employed for producing wetting angles in vacuum and in gaseous environment.
- Size sensitivity of water droplet on silica slab.

Simulation Details
- We investigated the SPC, TIP3P, and TIP4P water model for use in our simulation environment.
- We select TIP3P model for simulating water droplet for the current set of analysis.

Results & Discussion

2.5 nm Diameter Water Droplet

![Image](image1)

2.5 nm Diameter Water Droplet

![Image](image2)

5 nm Diameter Water Droplet

![Image](image3)

5 nm Diameter Water Droplet

![Image](image4)

- We seek to validate our models through previous literature. A previous study had concerned a Q3 slab, derived from alpha-cristobalite silica.
- As we move forward, we will both conduct experimental studies at the CCM and find more references to which our model can be validation.

Future Work
- Simulation of water droplets on silica in Nitrogen environment
- After careful validation of the Silica, Nitrogen, and Water models, we aim to move forward by developing more accurate models to validate the Silica-wetting angle, then more forward to Silane.
- We will Validate Silane chemistries such as GPS and APS. Along with this, a ML model will derive new Silanes.

Our silica slab utilized the OPLSAA Force Field derived parameters from PolyParGen.
Silica slab consists of an H-bond density of ~8 nm⁻².

Molecular Dynamics Model of Hydroxylated Q2 Silica Slab

Contact angle (Degree) evolution with respect to time (fs)

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