EFFECT OF SILANE DENSITY ON WETTABILITY OF SILANE-GRAFTED SILICA

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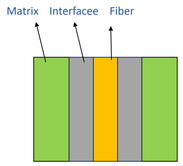
Introduction

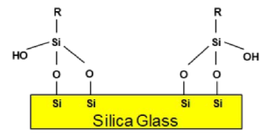
- Fiber-matrix adhesion is **critical** for transferring loads effectively and enhancing the overall strength and durability of composites.

  - 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.



Interphase region



Silane agent bonding to S-glass fiber.

- 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.

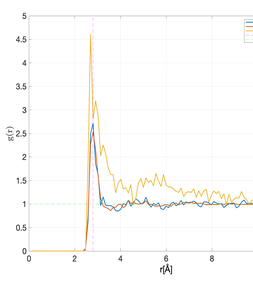
Simulation Details

- We investigated the SPC, TIP3P, and TIP4P water model for use in our simulation environment.

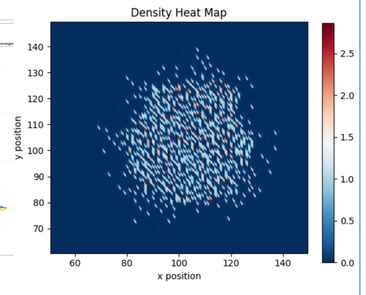
Model:	SPC	TIP3P	TIP4P
Accurate RDF Plot	✓	✓	✗
Shape Retention at STP	✗	✓	✓

Water model suitability result for water droplet when performed with SPC, TIP3P and TIP4P

We select TIP3P model for simulating water droplet for the current set of analysis.



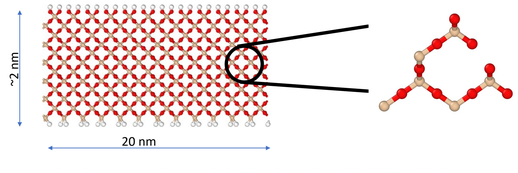
RDF Plots of MD Water models?: TIP3P: Red, SPC: Blue, TIP4P: Yellow.



Density map for TIP3P 5 nm diameter water droplet showcasing continuity

Our silica slab utilized the OPLSAA Force Field derived parameters from PolyParGen.

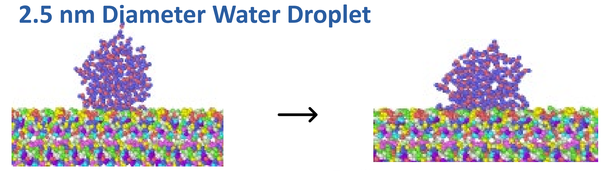
Silica slab consists of an H-bond density of ~8 $nm^{-2.}$



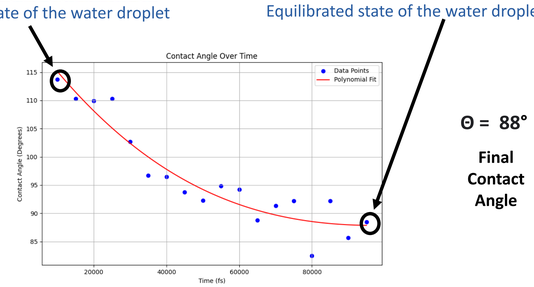
Molecular Dynamics Model of Hydroxylated Q2 Silica Slab

Results & Discussion

2.5 nm Diameter Water Droplet



Initial state of the water droplet → Equilibrated state of the water droplet

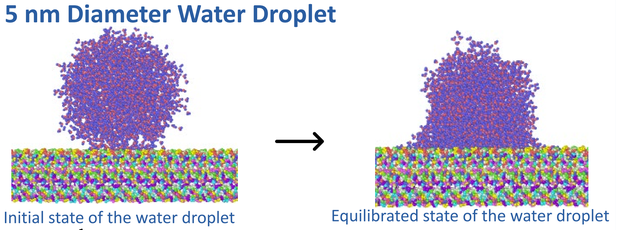


Θ = 88°

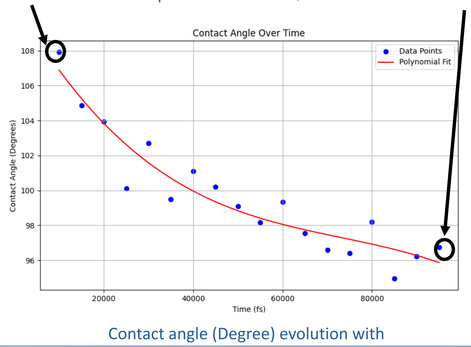
Final Contact Angle

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

5 nm Diameter Water Droplet



Initial state of the water droplet → Equilibrated state of the water droplet

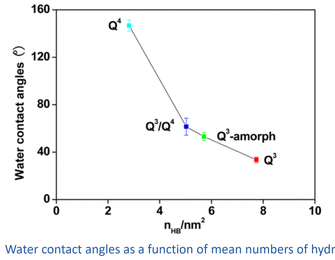


Θ = 96°

Final Contact Angle

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

- The cases shown above represent a subset of our work, with a contact angle analysis over 100,000 fs.
- We observe the slow decline and then variation in a quasi-equilibrium state.



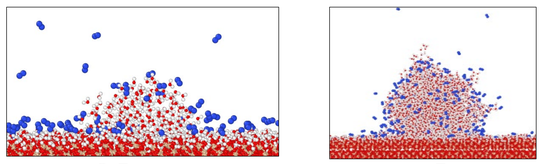
Referenced from: Water Contact Angle Dependence with Hydroxyl Functional Groups on Silica Surfaces under CO2 Sequestration Conditions by Chen et. al

Water contact angles as a function of mean numbers of hydrogen bonds per nm2 for silica–CO2 saturated water interaction.

- 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

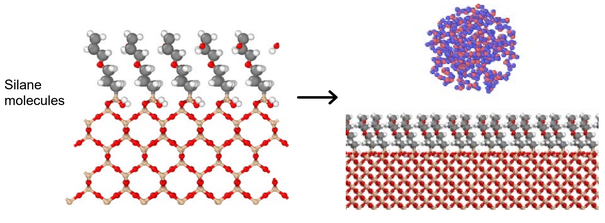
- Simulation of water droplets on silica in Nitrogen environment



2.5 nm **5 nm**

We are establishing a scripted-methodology for calculation of the Contact Angle in the 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.



GPS-grafted Silica is shown above, with a water droplet above representing the next step of our simulations

Acknowledgements

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