Organisation of Water and Alcohol Mixtures at the Interface with Solids

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Background

Alcohol in water is one of the fundamental liquid mixtures found in countless chemical and biological processes, where its behavior at interfaces is of interest to many industrial fields from fuel cells to surface treatments.

The aim of this project is to investigate the formation of a stable, solid hydrogen-bonded assembly of water and alcohol molecules at hydrophobic interfaces. The mere existence of such structures on these interfaces is surprising and completely novel.

Novel Structures

Our results prove that it is also possible to create monolayers of water with more complicated monohydric alcohols.

Monohydric Alcohols

- Ethanol
- 1-Propanol
- 2-Propanol

These show a high degree of polymorphism with multiple structures forming in a close proximity, some of which show clear sub-features.

AFM in liquids

- Atomically sharp tip attached to a cantilever which undergoes deflections when near to surfaces that can be measured in using a reflected laser beam projected onto a photodetector (see Fig. 1).
- Operate in dynamic mode where the tip oscillates to reduce lateral forces, preserve the surface and increase resolution.

Molecular Arrangements

Simulations suggest that at the interface molecules like to orientate themselves into ‘squares’ of 2 water and methanol molecules which then combine in 1D to form wires [1].

The interference between the periodicity of the HOPG and the repeated unit of the wires creates a supramolecular Moiré pattern.

The Big Questions

1) What are the structural differences between the monolayers we observe? Especially with those that show substructures and those that don’t.

2) Why do polyhydric alcohols form structures with similar Moiré patterns to that of monohydric alcohols?

The Future

We are currently performing Molecular Dynamics simulations to look at interfacial liquid behavior.

Moving on from this we will be interested in:

- Using Differential Scanning Calorimetry to investigate the nucleation.
- Replacing the water with heavy water (different hydrogen bonding properties) to investigate its importance within the structures.
- Influencing the formation of structures using electric potentials.

References