

Ice, ice maybe?

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There are few molecules, if any, more important than water. Yet remarkably little is known about how it interacts with solid surfaces, particularly at the all important atomic-level. This is true despite widespread general interest and compelling environmental and economic incentives. For example, water-solid interactions play a crucial role in the activity of fuel cells, the chemistry of the atmosphere, global warming, corrosion, catalysis, the operation of membranes, and so on. In this talk I will discuss some of our recent work in which we have been using classical and quantum molecular dynamics approaches as well as advanced electronic structure methods to better understand the structural and dynamical properties of water-solid interfaces. This will include work focused on understanding the formation of ice [1-4] and confined water in nanocapillaries [5].

References:

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