



The Role of Interfacial Water on Water Desalination, Hydrates Management, and Oil & Gas Production

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Abstract

The molecular structure of interfacial water, and in particular of the electric double layer, is known to determine the outcome of a number of physical processes, including the dissolution of minerals, corrosion, and perhaps even the biological activity of enzymes. Our research group has employed massive molecular simulation studies to quantify how interfaces, in particular wet ones, determine the outcome of processes of vast societal importance. In this presentation we will explore how water adsorption within clays can affect the transport of natural gas through shale formations, how water and CO₂ affect the mobility of hydrocarbons through silicates, how designing appropriately carbon-based electrodes could lead to new processes for water desalination, and finally how hydrates particles assemble within hydrocarbon systems. We will discuss how experimental information, obtained via appropriate collaborations, could be used to validate our predictions and perhaps lead to advancements in all the processes just discussed.