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Interfaces of methanol:water mixtures with an OTS-coated substrate probed by sum-frequency vibrational spectroscopy[1] WEITAO LIU, LUNING ZHANG, Y. R. SHEN, Physics Department, University of California at Berkeley — Aqueous solutions of short chain alcohols are important reagents in organic chemistry, and their physical and chemical properties at hydrophobic interfaces play key roles in many applications. To study their interfacial structures at the molecular level, we applied sum-frequency vibrational spectroscopy (SFVS) to the interfaces of methanol-water mixtures with an octyltrichlorosilane (OTS)-covered silica as model systems. From the methanol CH3 symmetric stretching mode, we deduced the interfacial coverage and orientation of methanol molecules vs. its molar concentration, and studied the hydrogen-bonding property of methanol with neighboring molecules. It appeared that methanol molecules adsorbed at the interfaces with the same average orientation at all concentrations. From the dangling-OH stretching mode of water molecules, we observed the correlation between the methanol surface number density and the water free OH bonds. Ab initio calculations were used to help investigate the interfacial structures of hydrogen-bonded species.

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Weitao Liu
Physics Department, University of California at Berkeley

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