

Abstract Submitted  
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**Hydrophobic dependence of molecules at the liquid/solid interface as studied with infrared-visible sum frequency generation spectroscopy** BRYAN HSU, VERONIQUE LACHAT, GABOR SOMORJAI, MOHSEN YEGANEH, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF CALIFORNIA, BERKELEY COLLABORATION, CORPORATE STRATEGIC RESEARCH, EXXONMOBIL RESEARCH AND ENGINEERING COMPANY COLLABORATION — We report IR-vis SFG spectra obtained at the interface of liquids with hydrophobic and hydrophilic solid surfaces. The hydrophilic and hydrophobic surfaces used were sapphire and a dense methyl-terminated sapphire surface from chemically bonded octadecyltrichlorosilane (OTS), respectively. Orientation calculations of SSP (IR, vis, and SF polarizations) and SPS polarizations of acetonitrile on the OTS and sapphire showed tilt angles of approximately 90 and 40 degrees, respectively. The CD3 symmetric stretch of methanol (d4) at OTS and sapphire showed a blue-shift for the latter but no shift for the former when compared to FTIR of the bulk liquid. This may be due to changing H-bonding characteristics with methanol orienting its hydroxyl end towards sapphire and away from OTS. PPP spectra of n-heptane (d16) and n-hexadecane (d34) showed weaker intensity CD3 antisymmetric stretches on sapphire compared to OTS, with a larger decrease for n-hexadecane. This can be interpreted as the hydrocarbons curling away from sapphire more so than OTS, especially with n-hexadecane.

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