

Vibrational SFG Spectra of *n*-Octadecyltrichlorosilane Monolayers Chemisorbed on SiO₂-deposited CaF₂ Substrates

○Adchara Padermshoke^{1,2}, Masato Ara³, Hirokazu Tada⁴, Taka-aki Ishibashi^{1,2}

¹ Center for Quantum Life Sciences, Hiroshima University, ² Graduate School of Science, Hiroshima University, ³ Institute for Nanoscience Design, Osaka University, ⁴ Graduate School of Engineering Science, Osaka University

Introduction. Infrared (IR)-visible/UV sum-frequency generation (SFG) spectroscopy is a method for measuring vibrational spectra of interface molecules. Because only surface or interface species give a resonant contribution to SFG signal, the technique is highly surface-specific and has been developed into a very powerful surface analytical tool. Aiming to measure SFG spectra of organic monolayers silanized on solid surfaces in aqueous environment, we have developed a new type of substrates that allow silanization and are transparent over a broad range of the IR probe. The silanized monolayers are robust, chemically stable, and can serve to surface-immobilize various types of biological molecules.

Experimental. The newly developed substrates comprise a thin SiO₂ layer (a few hundreds nanometer scale) overlying a CaF₂ (1 mm) plate. *n*-Octadecyltrichlorosilane (OTS) monolayers were chemisorbed onto pure SiO₂ and SiO₂/CaF₂ substrates under the same

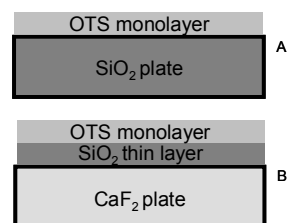


Fig. 1 OTS on A) SiO₂ and B) SiO₂/CaF₂ substrates.

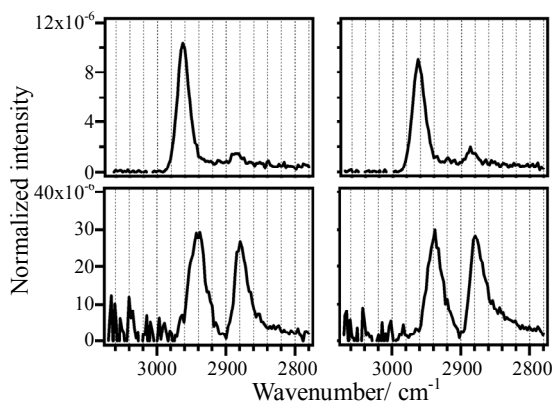


Fig. 2 SFG spectra of OTS on SiO₂ (left column) and SiO₂/CaF₂ (right column) substrates measured with ppp- and ssp-polarization combinations.

silanization condition. Fig. 1 depicts the layouts of the OTS samples on the two types of substrates. The SFG spectra were measured with ppp (SFG, visible, IR)- and ssp-polarization combinations.

Results and Discussion. Fig. 2 shows the normalized SFG spectra of the OTS monolayers on the SiO₂ and SiO₂/CaF₂ substrates. The spectral features obtained from the two samples are essentially identical for both polarization modes. Three peaks at 2965, 2940, and 2880 cm⁻¹ are dominant, all

of which are attributed to the CH stretching ($\nu(\text{CH})$) modes of the terminal methyl groups. Because the $\nu(\text{CH})$ bands of the methylene groups in all-*trans* alkyl chains are SFG inactive, these results suggest that the OTS molecules on both types of substrates are oriented in the same all-*trans* conformation, indicating the usability and efficiency of the SiO₂-deposited CaF₂ substrate.