FT-RAIRS AND DFT STUDIES OF HYDROGEN BONDING FORMATION IN THE CARBOXYLIC ACID TERMINATED THIOLATE MONOLAYERS ON AU SURFACE

LICHANG WANG, YANPING CAO, QINGFENG GE, and DAN J. DYER, *Department of Chemistry and Biochemistry, Southern Illinois University, Carbondale, IL 62901*; ,.

The formation of hydrogen-bonding network in the carboxylic acid terminated organic thiolate monolayer on gold (SAM) have been studied and characterized by the Fourier Transform Reflection-Absorption Infrared Spectroscopy (FT-RAIRS) and Density Functional Theory (DFT) calculations. A difference is observed in the formation of hydrogen bonds between the SAMs formed by the odd and the even number of carbon atoms. Monolayers with an odd number of carbon atoms exhibit a much stronger carbonyl stretching peak, associated to the lateral hydrogen bonding, than the monolayers with an even number of carbons atoms. The DFT calculations showed that the lateral hydrogen bonds can be easily formed in the SAMs with an odd number of carbon atoms while both the lateral hydrogen bonds and the dimer hydrogen bonds are energetically feasible in the SAMs with an even number of carbon atoms. Furthermore, DFT results showed that different C=O orientations in the even- and odd-carbon systems are the cause of the difference observed from the FT-RAIRS measurement.