The electronic structure and polymerization of a self-assembled monolayer DANQIN FENG, DAVID WISBEY, University of Nebraska-Lincoln, YIAN TAI, Universität Heidelberg, YAROSLAV LOSOVYJ, Center for Advanced Microstructures and Devices, MICHAEL ZHARNIKOV, Universität Heidelberg, PETER DOWBEN, University of Nebraska-Lincoln — Irradiation-induced modifications of electronic structure in the monomolecular insulator [1,1’:4’,1”-terphenyl]-4,4”-dimethanethiol (TPDMT) films have been investigated by photoemission and inverse photoemission. A dominant effect is cross-linking of the TPDMT film, which result in a quasipolymeric material with a smaller gap between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) but improved the dielectric properties. The cross-linking processes are also accompanied by changes in molecular orientation. The photoemission intensities of organic molecular layers generally obey the Debye-Waller temperature dependence but not always. With the example of a monomolecular film formed from [1,1’:4’,1”-terphenyl]-4,4”-dimethanethiol, we show that pronounced deviations from Debye-Waller temperature behavior are possible and are likely caused by temperature dependent changes in molecular orientation.

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