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**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.

Danqin Feng  
Dept. of Physics and Astronomy and the Center for Materials Research  
and Analysis, University of Nebraska-Lincoln, Lincoln, NE 68588-0111

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