

**O 82: Poster Session - Organic Molecules on Inorganic Substrates: Networks and Overlayers**

Time: Wednesday 18:15–20:00

Location: P2/EG

O 82.1 Wed 18:15 P2/EG

**Surface properties of en-APTAS SAMs on ZnO surfaces**

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Surface functionalization of ZnO nanowires with N-[3-(trimetoxysilyl)propyl]ethylenediamine (en-APTAS) self-assembled monolayers (SAMs) provides the base for an NO<sub>2</sub> gas sensor with high sensitivity and selectivity [1]. For a better understanding of the attachment of en-APTAS to the ZnO substrate, a comparative AFM, AES and XPS study of the chemical functionalization of undoped Zn-polar ZnO(0001) and nonpolar ZnO(11-20) single crystal surfaces with en-APTAS SAMs has been carried out. Monolayer films are readily deposited on ZnO(0001) by dip coating, while complete monolayer wetting of ZnO(11-20) was not achieved so far. An anomaly of the SiLVV/SiKLL Auger line intensity ratio for the Si atoms of the adsorbed en-APTAS layer is observed on both substrates. Possible implications of this anomaly and of incomplete hydrolysis of en-APTAS for the molecular adsorption geometry are discussed.

[1] M. W. G. Hoffmann et al., *Adv. Mater.* 26, 8017 (2014)

N. Majid would like to thank the Ministry of Research, Technology and Higher Education of the Republic of Indonesia (RISTEKDIKTI) for the RISETPro Ph.D. scholarship and Indonesian-German Centre

for Nano and Quantum Technologies (IG-Nano) for support.

O 82.2 Wed 18:15 P2/EG

**Surface-templating effect in the self-assembly of carboxyl-**

**functionalized bridged triphenylamine molecules** — •KEVIN DHAMO<sup>1</sup>, TOBIAS MÜLLER<sup>1</sup>, MARTIN GURRATH<sup>1</sup>, JIA LIU<sup>2</sup>, MIRUNALINI DEVARAJULU<sup>2</sup>, SABINE MAIER<sup>2</sup>, and BERND MEYER<sup>1</sup> — <sup>1</sup>Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — <sup>2</sup>Department of Physics, FAU Erlangen-Nürnberg

Since carboxyl groups form strong hydrogen bonds, one would expect that self-assembly of carboxyl-functionalized molecules is dominated by molecule–molecule interactions. However, in STM and AFM studies of carboxyl-substituted dimethylene-bridged triphenylamine (CDTPA) molecules the formation of very different networks was observed for Au(111), NaCl(001) and KBr(001) substrates. By using density-functional theory (DFT) calculations we analyze in detail the molecule–substrate and the molecule–molecule interactions for the different binding motifs. We show how site-specific interactions and enhanced van der Waals attraction between the molecules at denser packing stabilize alternative network structures depending on the lattice constant of the substrate. The possibility to tune self-assembly of organic molecules via the substrate lattice constant offers another degree of freedom for the rational design of functional molecular structures on surfaces.