

O 24: Semiconductor Substrates: Adsorption

Time: Monday 17:30–18:30

Location: WIL C307

O 24.1 Mon 17:30 WIL C307

Conductivity of a two-dimensional hole gas on diamond — ●DENNIS OING, NICOLAS WÖHRL, MARTIN GELLER, and AXEL LORKE — Universität Duisburg-Essen

Diamond is a material with promising properties like robustness, high thermal conductivity and high electric breakdown field. Because of the large band gap of 5.45 eV, diamond shows a low intrinsic charge carrier density at room temperature. However, a two-dimensional hole gas can be established on the surface by hydrogen termination and accumulation of an adsorbate layer.

We have produced a two-dimensional hole gas (2DHG) on chemical vapor deposition (CVD)-grown diamond through a hydrogen plasma treatment with varying parameters. This 2DHG is characterized using current-voltage (I-V) measurements and temperature-dependent Hall experiments. The Hall measurements reveal a p-type conductivity with a charge carrier density of $2 \cdot 10^{13} \text{ cm}^{-2}$ and a mobility of $60 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at room temperature. The temperature is varied in the range from 4.2 K up to 325 K, and we find a maximum of the mobility of $84 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at 230 K.

O 24.2 Mon 17:45 WIL C307

Chemoselective adsorption of functionalized cyclooctynes on silicon — MARCEL REUTZEL¹, NIELS MÜNSTER¹, MARCUS A. LIPPONER¹, CHRISTIAN LÄNGER², ULRICH HÖFER¹, ULRICH KOERT¹, and ●MICHAEL DÜRR² — ¹Philipps-Universität, 35037 Marburg — ²Justus-Liebig-Universität, 35392 Giessen

The high reactivity of the silicon dangling bonds presents a major hindrance for chemoselective attachment of bifunctional organic molecules on Si surfaces, the first basic reaction step for the controlled organic functionalization of silicon. Due to the high reactivity of the dangling bonds, each functional group of a bifunctional molecule adsorbs with an initial sticking coefficient close to unity and thus the final adsorption product will typically consist of a mixture of molecules adsorbed via different functional groups.

We overcome this problem employing cyclooctyne as the major building block of our strategy [1]. Using XPS and STM, cyclooctyne derivatives with different functional side groups are shown to react on Si(001) selectively via the strained cyclooctyne triple bond while leaving the side groups intact. The achieved selectivity originates from the distinctly different adsorption dynamics of the separate functionalities: A direct adsorption pathway is demonstrated for cyclooctyne as opposed to the vast majority of other organic functional groups. The latter ones react on Si(001) via a metastable intermediate, which makes them effectively unreactive in competition with the direct pathway of cyclooctyne's strained triple bond.

[1] Reutzet et al., J. Phys. Chem. C **120** 26284 (2016).

O 24.3 Mon 18:00 WIL C307

Ab initio thermodynamics of adsorbed atomic H at ZnO (10 $\bar{1}$ 0) — ●MARIA E. STOURNARA¹, SERGEY V. LEVCHENKO¹,

SANTIAGO RIGAMONTI², MARIA TROPPEZ², OLIVER HOFMANN³, PATRICK RINKE⁴, CLAUDIA DRAXL², and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der MPG, Berlin, DE — ²Faradayweg 4-6 — ³Technische Universität Graz, Graz, AT — ⁴Aalto University, Helsinki, FI

Zinc oxide (ZnO) is a highly multifunctional material with unique properties and a wide range of applications. To understand atomic hydrogen adsorption on the thermodynamically stable (10 $\bar{1}$ 0) surface at realistic H chemical potentials, we combine a first-principles cluster-expansion model with *ab initio* atomistic thermodynamics. Our study reveals that at coverages below 6%, H atoms adsorb exclusively on surface O. At higher coverages, H adsorbs also on Zn, but there is an excess of O-H over Zn-H at all coverages, except 50% and 100%. Due to an interplay of long- and short-range electrostatic interactions, neighboring O-H/Zn-H pairs form chains along surface -O-Zn- rows, with each chain anchored at the excess O-H, in a wide range of (T, p_{H_2}). Any ordering that could occur due to the long-range repulsion between the excess O-H is destroyed at $T > 60$ K. Our results explain available experimental data and provide detailed microscopic understanding of the ZnO surface properties at realistic (T, p_{H_2}) conditions.—This work was supported by the Hybrid Inorganic/Organic Systems (HIOS) CRC of the DFG.

O 24.4 Mon 18:15 WIL C307

Nanopatterning of Group-V-Elements for Tailoring the Electronic Properties of Semiconductors by Monolayer Doping — ●PETER THISEN¹ and ROBERTO LONGO² — ¹Karlsruher Institut für Technologie (KIT), Institut für Funktionelle Grenzflächen (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — ²Department of Materials Science & Engineering, The University of Texas at Dallas, Richardson, Texas 75080, USA

The control of the electronic properties of semiconductors is primarily achieved through doping. Within this context, new techniques such as Monolayer Doping (MLD) represent a substantial improvement towards surface doping with atomic and specific doping dose control at the nanoscale. Here, we address the key questions that will ultimately allow to optimize the scalability of the MLD process. First, we show that dopant coverage control cannot be achieved by simultaneous reactions of several group-V-elements, but stepwise reactions make it possible. Second, using *ab initio* molecular dynamics, we investigate the thermal decomposition of the molecular precursors, together with the stability of the corresponding binary and ternary dopant oxides, prior to the dopant diffusion into the semiconductor surface. Finally, the effect of the coverage and type of dopant on the electronic properties of the semiconductor is also analyzed. Furthermore, the atomistic characterization of the MLD process raises unexpected questions regarding possible crystal damage effects by dopant exchange with the semiconductor ions, or the final distribution of the doping impurities within the crystal structure.