

## O 111: Nanostructured Surfaces and Thin Films II: 1D and 2D Systems (joint session O/CPP)

Time: Thursday 15:00–17:15

Location: WIL B321

O 111.1 Thu 15:00 WIL B321

**Edges in group-IV monochalcogenides: stability and electronic properties** — ●MAHDI GHORBANI-ASL and ARKADY V. KRASHENINNIKOV — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany.

The group-IV monochalcogenides including tin sulfide (SnS) and germanium sulfide (GeS) are layered semiconductors with an anisotropic crystal structure giving rise to several unusual physical properties. In this study, based on density functional theory combined with different dispersion corrections, we systematically investigated the structure, stability and electronic properties of monolayer and multilayer SnS and GeS with various possible stoichiometric and nonstoichiometric terminations of the edges. It was found that the (110) facet has the lowest energy and it is thus expected to be the most stable edge. We further demonstrated that nonstoichiometric edges can exist as they provide reconstructed structure or covalent interlayer coupling between layers, which lowers the formation energies of the edges. The results indicate that the stability of the edges generally decreases for higher facet indices. The electronic structure calculations showed that most of the studied compounds are semiconductors with a band gap in the range of 0.2 - 1.6 eV, depending on the crystallographic direction of the edge and its chemical termination. For both GeS and SnS nanoribbons, the band gap is smallest in the case of the (010) edge and largest for the (110) edge. The edge states are more pronounced in multilayer than monolayer nanoribbons.

O 111.2 Thu 15:15 WIL B321

**MoS<sub>2</sub> monolayers under cluster ion irradiation: a molecular dynamics study** — ●SADEGH GHADERZADEH, VLADIMIR LADYGIN, MAHDI GHORBANI-ASL, and ARKADY V. KRASHENINNIKOV — Institute of Ion beam Physics and Materials Research Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

Ion irradiation is a powerful method to tailor the properties of low-dimensional materials, and is thought to be particularly promising for patterning two-dimensional (2D) materials through tuning the energy, type, charge state of the incident particles and the supporting substrate. This tool is recently employed to tackle the important issue of controlled pore creation in 2D materials to be performed as filters for water desalination, gas sensing, etc. This aim requires a clear insight into the microscopic process which is yet to be fully understood. In this work, we use classical Molecular Dynamics (MD) simulations to shed light on the behavior of 2D materials under cluster ion irradiation, and specifically focus on the production and characterization of defects. To a great extent, the properties of the induced defects depend on the size and energy of the clusters, which has not been studied beyond graphene so far. In particular, we are focused on the response of MoS<sub>2</sub> monolayers, which have shown various exciting properties complementary to graphene, under cluster irradiation. Furthermore, we show that depending on the incident angle and energy of the clusters, sulfur atoms can be sputtered mainly from the top layer, creating unique opportunities for patterning MoS<sub>2</sub> monolayers.

O 111.3 Thu 15:30 WIL B321

**One-dimensional molecular chains of Quinacridone on Ag(100) and Cu(111): STM- and SPA-LEED-investigations** — ●NIKLAS HUMBERG<sup>1</sup>, RÉMI BRETTEL<sup>2</sup>, ALEXANDER ESLAM<sup>1</sup>, and MORITZ SOKOLOWSKI<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany — <sup>2</sup>University of Paris-Saclay, Institut des Sciences Moléculaires D'Orsay, France

One-dimensional molecular aggregates are of high interest because they often show specific and pronounced coupling effects for electronic excitations, e.g. in optical spectra. Here, we report a structural analysis of two such systems, quinacridone (QA) on Ag(100) and Cu(111), by STM and SPA-LEED.

On Ag(100) QA grows in homochiral domains of parallel one-dimensional chains at room temperature (RT), forming a metastable structure. Within these chains the molecules are parallel and linked pairwise via two hydrogen bonds. The distance between chains varies with coverage. After annealing at 500 K, a 2D commensurate heterochiral structure is formed. It consists of homochiral dimers forming periodically indented and closely packed chains. On Cu(111), QA

grows in similar fashion at RT, but compared to QA/Ag(100) the structure shows stronger disorder in form of kink-like defects in the chains. Annealing at different temperatures between RT and 600 K leads to different chain-like structures, that are stable at RT. The comparison to the similar system QA/Ag(111) [1] indicates that the structures of QA/Cu(111) at RT are determined by kinetic limitations.

[1] Wagner et al, J. Phys. Chem. C 2014, 118, 20, 10911-10920.

O 111.4 Thu 15:45 WIL B321

**Fabrication of highly regular Moth-Eye inspired Nanostructures to generate Anti-Reflective Surfaces** — ●LOUISE KAESWURM, ZHAOLU DIAO, JOHANNES HIRTE, KLAUS WEISHAUP, and JOACHIM SPATZ — Max-Planck-Institute for Medical Research, Jahnstr. 29, 69120 Heidelberg, Germany

We developed a possibility to create highly regular moth-eye inspired anti-reflective (AR) nanostructures on different substrates such as silica glass, sapphire, diamond and silicon. Although thin-film technology can solve reflection related problems to a certain extent, AR moth-eye nanostructures have many advantages.

The method proposed is based on block copolymer micellar lithography to apply an etching mask and reactive ion etching to nanostructure the surface. Compared to other fabrication methods, this approach is fast and easily scalable. The method is based on the principle of index matching: the generated nanostructures lead to the reported reduction of the reflectivity. For transparent substrates the transmission is severely increased, for non-transparent the absorption. Since nanopillars and bulk are the same material, mechanical stress is reduced enabling applications in the high-energy regime. I.e. laser systems and EUV technology can profit from such an AR treatment. Additionally, AR sapphire windows for endoscopes can improve the imaging quality and AR silicon enhances the efficiency of different electronic devices. Further developing the processes will enable the use of the full potential of such AR surfaces for a variety of applications ranging from electronics to medical and optical applications.

O 111.5 Thu 16:00 WIL B321

**Length dependent symmetry in narrow chevron-like graphene nanoribbons** — ●KOEN HOUTSMA<sup>1</sup>, MIHAELA ENACHE<sup>1</sup>, REMCO HAVENITH<sup>1,2</sup>, and MEIKE STÖHR<sup>1</sup> — <sup>1</sup>Zernike Institute for Advanced Materials, University of Groningen, Groningen, the Netherlands — <sup>2</sup>Stratingh Institute for Chemistry, University of Groningen, Groningen, the Netherlands

Graphene nanoribbons (GNRs) are an exciting material that has aroused much interest due to their excellent and tunable electronic properties. Using on-surface synthesis, narrow chevron-like GNRs, which host a mixture of armchair and zigzag edge terminations, were synthesized from the prochiral molecular building block 6,12-dibromochrysene on a Au(111) substrate [1]. An interesting property of these ribbons is the changing structural symmetry depending on the number of monomer units incorporated in the ribbon, where ribbons consisting of an odd and even number of monomers are point and mirror symmetric, respectively. In our research, we characterized the electronic properties of these GNRs using scanning tunneling spectroscopy, also in dependence of their length and parity.

[1] T.A. Pham et al., Small 13 (2017) 1603675.

O 111.6 Thu 16:15 WIL B321

**Chirality transfer to supported metal particles and within organic dye films** — ●NATALIE FEHN, ALEXANDER VON WEBER, MATTHIAS JAKOB, PHILIP STANLEY, ARAS KARTOUZIAN, and UELI HEIZ — Chair of Physical Chemistry, Department of Chemistry and Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Chirality - the absence of improper rotation axes within a structure or molecule - is a phenomenon known since the early 19th century and leads to optical activity of the substance such as optical rotatory dispersion and circular dichroism. The phenomenon plays an important role in medication, biochemistry, and fine chemicals and still opens many questions such as the origin of life. We are especially interested in the transfer of chirality from chiral surfaces to small metal particles and adsorbates, which is addressed via circular dichroism spectroscopy and second harmonic generation-circular dichroism spectroscopy. We

already observed induced circular dichroism in silver nanoparticles [1] and organic dye thin films [2]. Now, the question arises whether chirality can be introduced into metal clusters which may serve as catalysts in asymmetric heterogeneous catalysis [3].

[1] M. Jakob, A. von Weber, A. Kartouzian, U. Heiz *PCCP* **31** (2018), 20347-20351, DOI: 10.1039/c8cp02970a. [2] A. von Weber, P. Stanley, M., Jakob, A. Kartouzian, U. Heiz *J. Phys. Chem. C* **14** (2019), 9255-9261, DOI: 10.1021/acs.jpcc.9b01323. [3] A. Kartouzian *Chirality* **31** (2019), 641-657, DOI: 10.1002/chir.23113.

O 111.7 Thu 16:30 WIL B321

**Enhanced efficiency of graphene-silicon Schottky junction solar cell through inverted pyramid arrays texturation** — •JIAJIA QIU<sup>1</sup>, HUAPING ZHAO<sup>1</sup>, LONG LIU<sup>1</sup>, WENHUI MA<sup>2</sup>, and YONG LEI<sup>1</sup> — <sup>1</sup>Institut für Physik & IMN MacroNano\* (ZIK), Technische Universität Ilmenau, Ilmenau, Germany — <sup>2</sup>State Key Laboratory of Complex Nonferrous Metal Resources Clean Utilization, Kunming University of Science and Technology, Kunming 650093, China

Nanostructures of silicon are gradually becoming hot candidate due to outstanding capability for trapping light and improving conversion efficiency of solar cell. In this paper, silicon nanowires (SiNWs) and silicon inverted pyramid arrays (SiIPs) were introduced on surface of Gr-Si solar cell through silver and copper-catalyzed chemical etching, respectively. The effects of SiNWs and SiIPs on carrier lifetime, optical properties and efficiency of Gr-SiNWs and Gr-SiIPs solar cells were systematically analyzed. The results show that the inverted pyramid arrays have more excellent ability for balancing antireflectance loss and surface area enlargement. The power conversion efficiency (PCE) and carrier lifetime of Gr-SiIPs devices respectively increase by 62% and 34% by comparing with that of Gr-SiNWs solar cells. Finally, the Gr-SiIPs cell with PCE of 5.63% was successfully achieved through nitric acid doping. This work proposes a new strategy to introduce the inverted pyramid arrays for improving the performance of Gr-Si solar cells.

O 111.8 Thu 16:45 WIL B321

**Spatial Extent of Surface Photovoltage in the Vicinity of Individual Plasmon Excited Nanoparticles** — •KATHARINA ENGSTER, KEVIN OLDENBURG, KARL-HEINZ MEIWES-BROER, SYLVIA

SPELLER, and INGO BARKE — Institute of Physics, University of Rostock

The investigation of photophysical processes of heterogeneous systems largely relies on local probing techniques [1]. For plasmon assisted electron-hole generation a key property is the size of the region that is affected by enhanced charge carrier density which is accessible via the local surface photovoltage (SPV). Here we present SPV studies of single resonantly excited Ag clusters [2] on Si(100)-(2x1) measured by energy-resolved two-photon photoemission electron microscopy (2PP-PEEM). Analysis of the distance dependence from the particles reveals an enhanced plasmon induced charge carrier density which decays on the scale of 1  $\mu\text{m}$ . This observation is corroborated by comparing spatially averaged SPV for different particle densities. We envision opportunities in the context of plasmon enhanced solar cells, particularly regarding the choice of optimal particle concentrations.

[1] K. Sell *et al.*, *Phys. Stat. Sol. (b)* **247**, 1087 (2010).

[2] K. Oldenburg *et al.*, *J. Phys. Chem. C* **123**, 1379 (2019).

O 111.9 Thu 17:00 WIL B321

**Supramolecular nanopatterns of arylenes and arylen-alkynyls: Addressing the third dimension** — GEORGIY POLUEKTOV, TRISTAN J. KELLER, JOSHUA BAHR, DAVID A. HOFMEISTER, ANNA KRÖNERT, ANNA JOCHEMICH, DIRK LAUX, DANIEL KALLE, SEBASTIAN HENZEL, STEVEN BECKER, •STEFAN-SVEN JESTER, and SIGURD HÖGER — Kekulé-Institut für Organische Chemie und Biochemie der Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Arylenes and arylen-alkynyls that carry long alkoxy side chains physisorb at the solid/liquid interface on graphite (HOPG). The resulting two-dimensional (2D) supramolecular nanopatterns have periodicities in the order of 3 nm to 10 nm and are *in situ* imaged by scanning tunneling microscopy (STM) with submolecular resolution. The electronic and mechanic decoupling of the active units in such systems from (i) the substrate surface and (ii) adjacent species within the nanopatterns is essential for a single-molecule functionality similar to systems in a solution. Here, we report on bicycphanes as well as shape-persistent stars and macrocycles, all carrying anchor groups that point along the surface normal.