

O 23: Poster Monday: Nanostructures 1

Time: Monday 18:00–20:00

Location: P4

O 23.1 Mon 18:00 P4

An Atomic Boltzmann Machine capable of Self-Adaption — BRIAN KIRALY¹, ELZE J. KNOL¹, ●WERNER M.J. VAN WEERDENBURG¹, HILBERT J. KAPPEN², and ALEXANDER A. KHAJETOORIANS¹ — ¹Institute for Molecules and Materials, Radboud University Nijmegen, the Netherlands — ²Donders Institute for Neuroscience, Radboud University Nijmegen, the Netherlands

A grand challenge in creating materials with brain-like functionality is understanding multi-well systems. Such multi-well landscapes are linked to energy-based machine learning models, often based on Ising spins. However, the typical short-ranged exchange coupling of Ising spins in real materials prohibit the connectivity required for multi-well landscapes. Therefore, understanding how to create multi-well systems and link these to attractor network models is vital [1].

We present an atomic Boltzmann machine capable of self-adaption using single Co atoms on Black Phosphorus (BP). Using the concept of orbital memory in Co atoms [2], we design a tunable multi-well energy landscape by patterning atoms with atomic manipulation in a scanning tunneling microscope (STM). By electrically gating the structure with the STM tip, we allow the dynamical exploration of its configurations. Due to the anisotropic BP, we find two different timescales that emulate a fast "neural" and a slow "synaptic" timescale. We demonstrate the self-adaption of the synaptic weights to electrical stimuli and explore frequency-based input signals in new types of orbital memory.

[1] Kolmus et al., *New J. Phys.* 22 (2020);

[2] Kiraly et al, *Nat. Comm.* 9 (2018)

O 23.2 Mon 18:00 P4

Pulling individual polar molecular wires off of a surface — ●CHRISTOPHE NACCI and LEONHARD GRILL — Department of Physical Chemistry, University of Graz, 8010 Graz, Austria

The frictional properties of individual nanostructures are strongly influenced by the reduced size and low dimensionality. Accordingly, challenging experiments are required to measure them. Probing the mechanical response of individual nanostructures on chemically different surfaces opens the possibility to explore how the static and dynamic friction depends on the interplay between structural commensurability and chemical composition. Here, we report the vertical pulling of DAD molecular wires [1] off metal surfaces by non-contact atomic force microscopy (AFM), performed under ultrahigh vacuum and at low temperatures. These are polar wires with alternating donor (D) and acceptor (A) groups incorporated in their chemical structure. The aim is to probe the mechanical response of individual molecular wires by force spectroscopy. To furthermore explore the role of structural commensurability between polymers and surface, the polar wires are grown on a variety of different surfaces, from stepped and corrugated surfaces to ultrathin insulating NaCl films on metal surfaces.

[1] C. Nacci et al., *Nature Comm.* 6, 7397 (2015)

O 23.3 Mon 18:00 P4

Efficient Sieving Performance with Carbon Nanomembranes (CNMs) — ●YUBO QI, PETR DEMENTYEV, and ARMIN GÖLZHÄUSER — Bielefeld University, Bielefeld, Germany

Nanoporous membranes are promising candidates in ion transport and molecular separation; however, it is still a great challenge to achieve high permeability and selectivity. Carbon nanomembranes (CNMs) emerge as attractive materials for water purification, energy storage, and gas separation. In this work, we present facile CNMs fabrication from polycyclic aromatic hydrocarbons that are drop-cast onto arbitrary supports, including foils and metalized films. The electron-induced polymerization is shown to result in continuous sheets of various thickness, and the material is characterized by some spectroscopic and microscopic techniques. The permeation measurements with free-standing membranes reveal a high degree of porosity, and the water permeance ($\sim 10^{-4}$ mol m⁻² s⁻¹ Pa⁻¹) is four orders of magnitude higher than helium ($\sim 10^{-8}$ mol m⁻² s⁻¹ Pa⁻¹) with a membrane thickness of 3.0 nm. The ion transport properties were investigated via bias voltage applied across through CNMs. The nanomembrane showed the ability to sieve monovalent and divalent cations, selectivity of all cations follow the ordering K⁺ > Na⁺ > Li⁺ > Ca²⁺ > Mg²⁺. Functional CNMs fabricated from inexpensive precursors pave the way towards the rational design of 2D membranes for high efficient

separation.

O 23.4 Mon 18:00 P4

Structure of NbO Nanocrystals on the Nb(110) Surface — ●SAMUEL BERMAN¹, KUANYSH ZHUSSUPBEKOV¹, AINUR ZHUSSUPBEKOVA¹, BRIAN WALLS¹, KILLIAN WALSH¹, SERGEY I. BOZHKO^{1,2}, ANDREY IONOV², DAVID D. O'REGAN^{1,3}, and IGOR V. SHVETS¹ — ¹School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland — ²Chernogolovka — ³AMBER, the SFI Research Centre for Advanced Materials and BioEngineering Research, Dublin 2, Ireland

The properties of Niobium based devices are greatly influenced by the presence of surface oxygen. The highly stable NbO(111) overlayer on the Nb(110) surface is known to host a distinctive nanocrystal structure, as observed by scanning tunnelling microscopy. However the exact structure of this surface has remained a mystery. In order to understand this surface structure, we carry out density functional theory calculations, along with scanning tunnelling microscopy/spectroscopy and X-ray/ultraviolet photoelectron spectroscopy experiments. We propose a new model, contrary to those previously proposed in the literature. The nanocrystal pattern is ascribed to a subtle reconstruction in the surface layer which locally breaks the hexagonal NbO(111) symmetry, giving rise to modulations in the local density of states. Excellent agreement is found between our model and the observed experimental data. We also investigate the underlying reasons that the surface adopts this unusual structure.

O 23.5 Mon 18:00 P4

Helium Ion Microscopy of insulating Materials using Charge Compensation — ●MICHAEL WESTPHAL¹, NATALIE FRESE¹, YUBO QI¹, HIROYUKI TAKEI², PETR DEMENTYEV¹, ANDRÉ BEYER¹, and ARMIN GÖLZHÄUSER¹ — ¹Bielefeld University, Germany — ²Toyo University, Japan

Surface-sensitive imaging capabilities in nanotechnology have become increasingly important in recent years. While scanning electron microscopes (SEM) have become more powerful, they reach their limits when it comes to electrically insulating samples. The accumulation of charge carriers on the sample surface can lead to severe imaging artifacts which necessitates the application of conductive coatings. Helium ion microscopes (HIM) have the possibility to stabilize electric charges by using an electron flood gun to reveal nanoscopic sample features that would otherwise be covered by a conductive coating. In this contribution, we show the benefits of charge-compensated HIM imaging over conventional SEM imaging using the examples of SARS-CoV-2 virus particles [1], carbon nanomembranes from Aromatic Precursors without Headgroups, metal coated SiO₂- and carbon micro-spheres [2]. [1] N. Frese et al. , *Beilstein Journal of Nanotechnology* 12 172-179 (2021). [2] M. Wortmann et al., *Journal of Analytical and Applied Pyrolysis* Volume 161, January 2022, 105404.

O 23.6 Mon 18:00 P4

2D covalent organic frameworks from diboronic acids: the influence of the solvent — ●WENBO LU, ETHAN MALONE, MHAELA ENACHE, and MEIKE STÖHR — Zernike Institute for Advanced Materials, University of Groningen, Netherlands

Over the past years, two-dimensional (2D) covalent organic frameworks (COFs) have gained substantial interest for their use in nanopatterning, organic electronics, and as a basis for nanoreactors or molecular sieves. In particular, 2D COFs formed by polycondensation of boronic acids on surfaces have already yielded promising results [1, 2].

In this study, 2D COFs were synthesized by 1,4-benzenediboronic acid (BDPA) polycondensation on highly oriented pyrolytic graphite (HOPG) which resulted in the formation of a long-range ordered hexagonal molecular network. For the formation of the 2D COFs, a drop of BDPA solution was deposited onto HOPG, then placed in an autoclave and annealed at certain temperature. The structure and coverage of the 2D COFs was studied by scanning tunneling microscopy and atomic force microscopy under ambient conditions. In order to obtain both high quality as well as extended COFs, the influence of four solvents on the COF formation was studied. Our results provide guidance for obtaining high quality 2D COFs formed by boronic acid derivatives.

- [1] S. Spitzer et al., *Chemical Communications* 53 (2017) 5147.
 [2] J. F. Dienstmaier et al., *ACS Nano* 6 (2012) 7234.

O 23.7 Mon 18:00 P4

On-surface synthesis of narrow porous graphene nanoribbons — ●CHRISTOPH DOBNER¹, MAMUN SARKER², ADRIAN EBERT¹, ALEXANDER SINITSKII², and AXEL ENDERS¹ — ¹Physikalisches Institut, Universität Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany — ²Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE68588, USA

Fueled by the technological necessity to induce semiconducting properties in graphenic nanostructures, the search for strategies to manipulate their electronic properties has become an active field of research. Common control parameters that determine the band gap of graphene nanoribbons (GNR) are structural width, edge design and heteroatom doping. It has also been theoretically predicted that periodic vacancies can open up a band gap in to otherwise semimetallic 2D-graphene sheets. It is thus reasonable to expect that porosity could also contribute to the band structure of already semiconducting GNRs. In this work we present a strategy for the on-surface synthesis of porous GNRs using precursor. We will show that modified halogenation sites on the precursor molecules result in GNRs containing a periodic arrangement of vacancies along the ribbons backbones. Tunneling spectroscopy was used to determine the band edge locations and band gap width of such structures, revealing a increased band gap of 1.96 eV. Additional dI/dV mapping revealed that periodic electronic states are located at the edges and inside the backbone, induced by the porosity of the structures. Based on these findings a route towards considerably wider porous graphenic flakes will be discussed.

O 23.8 Mon 18:00 P4

Construction of a regular tessellation via bromine bond on a Ag(100) surface — ●WENCHAO ZHAO, NAN CAO, BIAO YANG, and JOHANNES V BARTH — Physics Department E20, Technical University of Munich, D-85748 Garching, (Germany)

Engineering 2D surface tessellations at the molecular level attracted major interest with the development of nanoscience and technology. To this end supramolecular self-assembly exploiting tailored molecular species and programmed intermolecular interaction are widely employed. Halogen bonds are promising for potential application due

to the σ -hole anisotropic charge distribution of halogen atoms^{1,2,3}. Herein, we address the behavior of ditopic bromine-terminated linear monomers on a Ag(100) surface at the molecular level, affording a tessellation guided by the surface symmetry. In the temperature range of 120 to 200 K, the building blocks form a porous nested grid structure stabilized by bromine bonds and molecule-substrate interactions. Two kinds of quad nodes are distinguished therein, involving a complex non-covalent bonding scheme. Interestingly, both nodes feature supramolecular chirality, entailing domains with both rectangular and trapezoid cavities. Our work introduces a new and complex surface tessellation scheme based on halogenated hydrocarbons on metal surfaces. References 1. G. Cavallo et al., *Chem. Rev.* 116, 2478-2601 (2016). 2. Z. Han et al., *Science* 358, 206-210 (2017) 3. Mallada et al., *Science* 374, 863-867 (2021)

O 23.9 Mon 18:00 P4

Graphitic nitrogen substitution in graphene nanoribbons — ●NICCOLÒ BASSI¹, FEIFEI XIANG¹, PASCAL RUFFIEUX¹, AKIMITSU NARITA², KLAUS MÜLLEN², and ROMAN FASEL¹ — ¹Empa-Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — ²Max Planck Institute for Polymer Research, 55124 Mainz, Germany

Graphene nanoribbons (GNRs), nanometer-wide strips of graphene, have attracted significant attention thanks to their tunable electronic properties originating from quantum confinement. A possible way to control these properties is through carbon substitution with heteroatoms, such as nitrogen. Despite a large number of theoretical studies, there are few experiments where controlled N substitution has been achieved. We report the on-surface synthesis on Au of two different types of nanoribbons containing N atoms from specifically designed heteroaromatic precursors. The chemical structures of the resulting ribbons were characterized using scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM). We demonstrate the high quality ribbons growth, which involves a facile C-N bond formation at temperatures below typical C-C reactions. The electronic properties were further investigated by scanning tunneling spectroscopy (STS), which revealed unoccupied states localized on N atoms that are absent in the undoped sections. These results open new perspectives for growing and studying novel types of GNRs with the possibility to fine-tune electronic properties by controlled heteroatom substitution.