Functional Thin Films and Surfaces
Room Palm 5-6 - Session MB3-MoM

Low-dimensional Materials and Structures

Moderators: Vladimir Popok, FOM Technologies, Denmark, **Kostas Sarakinos**, University of Helsinki, Finland

10:00am **MB3-MoM-1 Shape and Symmetry Engineering in Transition Metal Dichalcogenide Nanoribbons for Light Harvesting**, *Ganesh Ghimire, **Stela Canulescu [stec@dtu.dk]**,* Technical University of Denmark, Denmark **INVITED**

In this talk, I will discuss how controlling shape and symmetry at the nanoscale can fundamentally change how transition-metal dichalcogenides (TMDs) interact with light. By tailoring these materials into nanoribbon architectures, we can induce local symmetry breaking, tune excitonic behavior, and open new pathways for light harvesting and nonlinear optical response.

I will begin by introducing our alkali-assisted CVD approach for growing highly crystalline MoS_2 nanoribbons.[1,2] These nanoribbons can extend to tens of microns in length and naturally form monolayer–multilayer junctions within a single structure. This built-in structural gradient creates regions that either preserve or break inversion symmetry. As a result, we observe strong second harmonic generation and distinct excitonic emission localized at the nanoribbon edges. These symmetry-driven optical characteristics directly translate into improved device performance: individual nanoribbon photodetectors exhibit responsivities among the highest reported for TMD-based nanoscale photodetectors.

I will then expand the discussion to the bulk photovoltaic effect (BPVE), a mechanism that enables photocurrent generation in non-centrosymmetric crystals without the need for p–n junctions. I will show how engineered asymmetry in 3R-stacked MoS_2 and lithographically defined WS_2 nanoribbons leads to strong nonlinear optical response and shift-current generation. The resulting devices display large short-circuit current densities and measurable open-circuit voltages, underscoring the potential of symmetry-driven photovoltaic operation.

Overall, I will highlight how **nanoscale shape and symmetry engineering** serve as powerful design principles for next-generation optoelectronic and energy-conversion technologies. By deliberately breaking symmetry—through strain, stacking control, and dimensional confinement—we can create TMD architectures that harvest light more efficiently and exhibit enhanced nonlinear optical behavior. These findings position TMD nanoribbons as versatile building blocks for future light conversion, sensing, and photovoltaic applications.

References:

1. Ghimire, G. *et al.* Molybdenum Disulfide Nanoribbons with Enhanced Edge Nonlinear Response and Photoresponsivity. *Adv. Mat.* 35, (2023).

2. Miakota, D. I., Ghimire, G., Ulaganathan, R., Rodriguez, M. & Canulescu, S. A novel two-step route to unidirectional growth of multilayer MoS_2 nanoribbons. *Appl Surf Sci*. 619, (2023)

10:40am **MB3-MoM-3 Discovery of Goldene Comprising Single-atom Layer Gold; Prospects for Novel Noble Metallenes**, ***Lars Hultman [lars.hultman@strategiska.se]**,* Linköping University, IFM, Thin Film Physics Division, Sweden **INVITED**

The quest to make monolayer gold has hitherto been limited to a few atomic layers stabilized on or inside another material. The bonding nature of metals is the root cause to gold's tendency to take 3D shapes during all kinds of synthesis, like vapor-phase deposition or precipitation from solutions.

Through an innovative scheme, single-atom-thick 2D gold[1)], named *goldene*, has been exfoliated by wet-chemically etching away Ti_3C_2 layers from Ti_3AuC_2 nano-laminated MAX-phase[2), 3)] ceramic initially formed by substituting the Si layer in Ti_3SiC_2thin films with Au[3)]. The driving force for such exchange substitution lies in the eutectic nature of the Au-Si phase diagram. Etching-free the goldene sheets is made using a diluted form of the Murakami's reagent[5)]. Surfactant schemes are applied to hinder *goldene* sheets from coalescing with each other in water suspension. *Goldene* is observed by scanning transmission electron microscopy. A tendency for curling and agglomeration of*goldene* is observed, whereas *ab initio* molecular dynamics simulation shows that flat atomic layers are inherently stable. X-ray photoelectron spectroscopy reveals an Au 4f binding energy increase of 0.88 eV. Prospects for preparing *goldene* from a series of carbide and nitride MAX phases are also presented.Proposed applications for *goldene* include sensors and photocatalyst for water splitting during solar energy harvesting. The use of Au resources would be minimized due to the ultimate surface-area-to-volume ratio for *goldene*.

Isolated three-atomic-layer Au sheets – trilayer *goldene* – was recently reported by us by selectively removing the Ti_4C_3 sheets from $Ti_4Au_3C_3$, formed by Au-intercalated Ti_4SiC_3 thin films.[6)] Finally, this presentation will discuss ways to realize other noble-metal *metallenes*[7)] from thin-film or bulk-powder templates.

1. *Nature Synthesis*, **3** (April 16, 2024) 744-751

2. *MAX phases* are inherently nanolaminated hexagonal ternary metal carbides and/or nitrides with a general formula $M_{n+1}AX_n$, where M is a transition metal, A is a group 13-16 element, X is carbon and/or nitrogen, and n = 1, 2, 3,...

3. Review: M. Dahlqvist, M.W. Barsoum, J. Rosen, *Materials Today* **72** (2024) Jan/Feb, p. 1 https://doi.org/10.1016/j.mattod.2023.11.010

4. H. Fashandi, M. Dahlqvist, J. Lu, J. Palisaitis, S. Simak, I. Abrikosov, J. Rosen, L. Hultman, M.Andersson, A.Lloyd-Spetz, P.Eklund *Nature Materials* **16** (2017) 814

5. Potassium ferricyanide is combined with potassium hydroxide (or sodium hydroxide) and water to formulate Murakami's etchant.

6. Y. Shi, [...], L. Hultman*Sci. Advances***11**, eadt7999 (2025) 28 March 2025
S. Kashiwaya, Y. Shi, J. Rosen, L, Hultman, *2D Materials* **12** (2025) 033001

11:20am **MB3-MoM-5 Nanoporous TiO2 Thin Films by Helium-Assisted Sputtering for Noble-Metal-Free Hydrogen Sensing**, ***Stanislav Haviar [haviar@ntis.zcu.cz]**, Akash Kumar, Tomáš Kozák, Petr Zeman,* University of West Bohemia in Pilsen, Czechia

A large portion of magnetron-sputtered film applications targets the fabrication of highly compact, dense films. Textbook knowledge of thin-film growth delineates process windows that lead to "low-quality," non-compact morphologies. However, there are use cases where higher porosity or other forms of nanostructuring are advantageous—for example, when a large reactive surface area is desired. In this work, we discuss a modification of classical reactive sputtering in an Ar/O_2 mixture by introducing helium gas. Subsequently, we evaluate the resulting materials assembled as conductometric hydrogen gas sensors.

Titanium oxide films were deposited by conventional DC reactive sputtering, where helium replaced part of the Ar/O_2 working-gas mixture. The substoichiometric as-deposited films were post-annealed to achieve stable TiO_2. The introduction of helium promotes the formation of distinctive morphological features, which increase film porosity, as observed by electron microscopy.

We analyze the mechanisms involving reflected fast neutrals underpinning the emergence of nanoporous structures, supported by SEM imaging as well as structural characterization via XRD and Raman spectroscopy. We describe the evolution of the microstructure with annealing temperature and identify key processing parameters required to obtain porous yet stable films.

The application potential is then assessed by employing the films as conductometric hydrogen sensors. Films prepared by He-assisted sputtering show a several-fold increase in sensitivity to hydrogen without the addition of any noble metals.

Overall, controlled nanostructuring of thin films represents a promising route to engineer novel materials for gas sensing, and He-assisted deposition is one such approach.

11:40am **MB3-MoM-6 Large-Area Single-Crystals of Borophene on Square and Triangular Copper Surfaces: Synthesis and Characterization***, **Adrian Gozar [agzar@fairfield.edu]***, Fairfield University and Yale University, USA*; Ivan Bozovic,* Yale University and Shanghai Advanced Research in Physical Sciences, USA **INVITED**

The materials-by-design paradigm is based on synergistic efforts involving synthesis, characterization and advanced computation to ensure materials meet technological needs within a cost-effective framework. Borophene, a crystalline monolayer sheet, is envisaged to play an important role in this area because of its extraordinarily rich polymorphism. The multitude of potentially stable structures singles out borophene from all other two-dimensional materials and fuels hopes for obtaining on-demand structures with applications in flexible electronics, energy storage or catalysis.

We have used a unique ultra-high vacuum system for synthesis, by Molecular Beam Epitaxy, and in-situ characterization, by Low Energy Electron Microscopy, of micron-size borophene crystals on Cu(111) and Cu(100) substrates. Our real-time imaging capabilities provide information about the growth of faceted borophene islands up full monolayer coverage and also about phase-stability, evaporation and sub-surface dissolution. Combining low energy electron diffraction with scanning tunneling microscopy and ab initio theory allows us to resolve the crystal structures as triangular networks with vacancy ratios $\eta = 1/5$ for Cu(111) and $\eta = 1/6$ for Cu(100) surfaces. First-principles calculations indicate that charge transfer rather than covalent bonding, couples borophene to the underling Cu surfaces. The calculated electronic band structures host multiple anisotropic Dirac cones. Ex-situ scanning near-field optical microscopy data reveal dielectric contrast between borophene and substrates, showing that nano-optical tools provide new ways to access intrinsic electronic properties of these novel structures.

[1] R. Wu et al., J. Vacuum Sci. Tech. A 43, 042703 (2025)

[2] J. Zhao et al., Rev. Sci. Instrum. 96, 023907 (2025)

[3] A. Gozar et al., Nano Today 50, 101856 (2023)

[4] R. Wu et al., Nature Chemistry 14, 377 (2022)

[5] I. Bozovic, Nature Materials 21, 11 (2022)

[6] R. Wu et al., Nature Nanotechnology 14, 44 (2019)

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