## Monday Morning, May 20, 2024

### Functional Thin Films and Surfaces Room Town & Country A - Session MB4-MoM

2D Materials: Synthesis, Characterization, and Applications Moderators: Chih-Yen Chen, National Sun Yat-sen University, Taiwan, Ying-Hao Chu, National Tsing Hua University, Taiwan

# 10:00am MB4-MoM-1 Influence of Plasmonic Coupling and Size Effect on Photocatalysis of MoS<sub>2</sub>/Au Hybrid Nanostructures for Water Splitting, *Yi-Hsueh Chen* (t870116@gmail.com), J. Ruan, NCKU, Taiwan

Hydrogen energy is a clean and sustainable form of energy for our environment, serving as a viable alternative energy source that can be used without the production of greenhouse gases. Utilizing solar energy to split the water and generate hydrogen in the presence of photocatalysts is a promising and economic approach to address the current energy and environmental crisis.  $MoS_2$  has been recognized as the most efficient photocatalyst for hydrogen evolution among non-noble metals. In particular, MoS<sub>2</sub> nanosheets exposed lots of active sites for the attachment of proton and later reduction reactions, and the efficiency is better than nanoflowers or bulk morphology. However, the absorption wavelength of MoS<sub>2</sub> nanosheets is almost within the UV region, in addition to the challenge of high electron/hole pairs recombination rate. Visible light accounts for 95% of sunlight and UV light occupies only 5%. It is vital for photocatalysts to efficiently harvest visible light and avoid exciton recombination. The absorption of visible light is able to cause strong localized surface plasmon resonance (LSPR) of gold nanoparticles (AuNPs), which has been widely investigated to promote light absorbance. Nevertheless, the desired dispersion patterns of AuNPs for the optimization of plasmonic resonance are less achievable. As an approach to maximize the amount of energy absorbed from the sunlight, we aim to design and fabricate hybrid particles composed of AuNPs and MoS<sub>2</sub> nanosheets with the control of coupling effect among AuNPs and the size of AuNPs. We have successfully grown  $\mathsf{MoS}_2$  nanosheets directly on the (111) planes of gold nanoparticles to form the core-shell structure with controlled thicknesses. Furthermore, the extent of enhancement of plasmonic coupling for gold nanoparticles with different diameters, i.e. 16 nm and 38 nm has been verified. Through the achieved adjustment of edge-to-edge distances among AuNPs and the size of AuNPs, the required condition for the best plasmonic resonance to absorb visible light is able to be clarified and thus optimizes the hot electron transition from AuNPs to MoS<sub>2</sub>, which critically enhances desired hydrogen production.

10:20am MB4-MoM-2 Sputter Deposition of Hexagonal Boron Nitride Films, Minsuk Seo (seo3@llnl.gov), L. Bayu Aji, Lawrence Livermore National Laboratory, USA; Y. Tzeng, S. Kim, Stanford University, USA; Y. Zhou, L. Wan, C. Kim, B. Wang, T. Heo, L. Zepeda-Ruiz, Lawrence Livermore National Laboratory, USA; S. Chu, Stanford University, USA; S. Kucheyev, Lawrence Livermore National Laboratory, USA

Hexagonal boron nitride (hBN) films are attractive for several emerging energy-related applications. Extensive previous research has focused on the growth and properties of either ultrathin hBN films with thicknesses up to a few monolayers or cubic BN films. The synthesis of wafer-scale hBN films with controlled thickness above ~10 nm with desired properties remains a challenge. Here, we present results of our ongoing systematic study of polycrystalline hBN films with thicknesses in a wide range of 50-6000 nm deposited by several variants of reactive magnetron sputtering with a radiofrequency (RF) driven discharge. We describe how the plasma discharge characteristics and, hence, resultant major film properties can be controlled by the magnetron source design, the confining magnetic field, and process parameters such as the working gas pressure (influencing landing neutral atom ballistics and energetics), substrate temperature (adatom mobility), and substrate bias (bombarding ion energy). Even without epitaxy, with substrates held close to room temperature, hBN films are polycrystalline, characterized by a FWHM of the major E<sub>2g</sub> Raman vibrational mode (1370 cm<sup>-1</sup>) in the range of 40 – 100 cm<sup>-1</sup>, depending on deposition conditions. The FWHM reduces to ~30 cm<sup>-1</sup> when a higher deposition temperature of 600-800 °C is used. Interestingly, all as-grown films are polycrystalline (turbostratic, with asymmetrically stacked layers) rather than amorphous even for a high deposition pressure of 50 mTorr, characterized by low landing atom energetics. We also describe how these film growth and characterization experiments are guided by results of insitu plasma diagnostics.

This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA2734.

10:40am MB4-MoM-3 Advancing 2D Materials for Future Electronics: Selective Synthesis, Transferring Processes, and Device Integration, *Ching Yuan Su (cysu@ncu.edu.tw)*, National Central University, Taiwan INVITED Two-dimensional (2D) materials like graphene and transition metal dichalcogenides (TMDs) have attracted significant attention due to their exceptional electrical properties, holding promise for next-generation nanoelectronics. However, integrating 2D materials into IC devices presents challenges, including precisely controlled synthesis methods, defect-free transfer processes, and back-end-of-line (BEOL) device integration.

In this talk, I will discuss advancements in selectively seeding growth of high-quality 2D materials on insulating substrates using a new precursor and advanced process. Additionally, an efficient and reliable method for the wafer-scale transfer of graphene and other 2D materials, ensuring integrity and cleanliness, will be presented. Finally, I will highlight the concept of a heterogeneously integrated 3D-IC, combining a 2D-based field-effect transistor (FET) with high-performance memory, showcasing the potential for BEOL and monolithic integration of 2D-based 3D-ICs.

11:20am MB4-MoM-5 Reduced Electrocatalytic potential of Nitrate to Ammonia through MoS<sub>2</sub> Deposited Carbon Felt based Flexible Electrode, *Prateek Sharma (prateeksharma1688@gmail.com), C. Liao, Y. Chang, D. Huang, W. Hsu, J. Huang, Y. Lai,* Ming Chi University of Technology, Taiwan The increasing need, for environment friendly and energy efficient methods to remove nitrate from water has prompted the investigation of inventive electrocatalytic techniques. This work highlights an approach to convert

electrocatalytic techniques. This work highlights an approach to convert nitrate into ammonia at low potential using carbon felt coated with Molybdenum disulfide (MoS<sub>2</sub>) nanosheets as a flexible electrode. The layered structure of MoS<sub>2</sub>, with exposed edge sites, provides active catalytic sites for the reduction reactions. This enhances the catalytic activity compared to other materials, contributing to more efficient nitrate ion degradation, making it a potential candidate for sustainable water treatment.MoS<sub>2</sub> can be deposited on flexible substrates, such as carbon felt, creating flexible electrodes.the flexible nature of the MoS2-deposited carbon felt electrode enhances the catalytic activity, allows for easy integration into existing water treatment systems, providing adaptability and scalability for practical applications. This research contributes towards the formation of efficient MoS<sub>2</sub> nanosheets as catalyst material for the advancement of electrocatalysis for sustainable water treatment but also underscores the significance of flexible electrodes in enhancing the adaptability and efficiency of the nitrate to ammonia conversion process. The findings presented in this conference aim to foster discussions and collaborations towards the development of energy-efficient and environmentally friendly technologies for nitrogen removal from water sources.

**Keywords:** Nitrate ion reduction, Electrocatalysis, Flexible electrode, Electrodeposition, MoS<sub>2</sub> nanosheets

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