Frontiers of New Light Sources Applied to Materials, Interfaces, and Processing Focus Topic
Room A124-125 - Session LS+HC+SS-ThM

Frontiers of Time-resolved Techniques for Energy & Catalysis Highlight Session

Moderator: Jessica McChesney, Argonne National Laboratory

11:00am **LS+HC+SS-ThM10 How to Probe Solid/Liquid Interfaces using Standing-wave Photoemission?**, ***Slavomir Nemsak***, Lawrence Berkeley National Laboratory; *H. Bluhm,* Fritz Haber Institute, Germany; *C.S. Fadley,* University of California, Davis

A great efforts have been made in the development of *in-situ* and *operando* experimental methods in the last two decades, with ambient pressure photoelectron spectroscopy being one of the most profound examples [1]. In combination with advanced techniques, such as standing wave excitation, an unprecedented depth resolution across operating interfaces can be obtained, providing valuable information on processes governing interfacial behavior.

With the excellent depth selectivity and sensitivity to chemistry and electrostatic gradients, standing wave ambient pressure photoelectron spectroscopy is exploited to probe two different solid/liquid interfaces relevant to energy research, electrochemistry, and atmospheric and environmental science [2,3]. Liquid layers are prepared either by water adsorption in a saturated vapor ambiance or using a so-called meniscus method, in which the sample is pulled out of a liquid reservoir leaving a thin liquid film on the sample's surface. The latter experimental configuration allows also for the *operando* electrochemistry [4]. The outlook and future developments of the technique will be also discussed.

[1] D.E. Starr et al., *Chem. Soc. Rev.***42**, 5833 (2013).

[2] S. Nemšák et al., *Nat. Comm.***5**, 5441 (2014).

[3] O. Karslıoğlu et al., *Faraday Discuss.***180**, 35 (2015).

[4] S. Axnanda et al., *Sci. Rep.***5**, 9788 (2015).

11:20am **LS+HC+SS-ThM11 *In situ* Spectroscopy of Synthesis of Next-Generation Cathodes for Batteries**, ***Feng Wang***, Brookhaven National Laboratory

There has been considerable interest in developing low-cost, high-energy electrodes for batteries. However, synthesizing materials with the desired phases and properties has proven difficult due to the complexity of the reactions involved in chemical synthesis. Additional challenge comes from the fact that synthesis is often undertaken under conditions and, hence, the process is hard to be predicted by theoretical computations. probing of synthesis reactions allows for identification of intermediates and determination of thermodynamic/kinetic parameters governing kinetic reaction pathways, thereby enabling synthetic design of materials with desired structure and properties. In this presentation, we will report our recent results from technique development and application to *in situ* probing and synthetic control of local structural ordering and stoichiometry during synthesis of next-generation cathode materials for lithium-ion batteries. Findings from this study, along with its implication to designing viable cathodes for practical use in batteries, will be discussed.

ACKNOWLEDGMENT. This work was supported by the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy, Vehicle Technologies Office, Contract No. DE-SC0012704.

11:40am **LS+HC+SS-ThM12 Structural Heterogeneity and Dynamics of 2D Materials Studied by Full-field X-ray Diffraction Microscopy and Ultrafast Surface X-ray Diffraction**, ***Haidan Wen***, Argonne National Laboratory **INVITED**

Transition metal dichalcogenides (TMD) at the two-dimensional (2D) limit have sparked great interests in both fundamental physics and devices applications. Surfaces and interfaces play an important role in t he most common setting, i.e., a monolayer crystal on a substrate, for studying 2D phenomena and device applications. However, the structural characterization with atomic accuracy in this form has been a challenge because the crystal size is usually small and transmission electron microscopy is difficult to apply. In this talk, we show microscopic insights of structural properties can be obtained in the space or time domain using newly developed multimodal full-field x-ray imaging and ultrafast surface x-ray scattering. In the first example, we demonstrate full-field x-ray diffraction imaging of a monolayer 2D material at the Advanced Photon Source. The structural variation across a TMD monolayer or heterostructure is spatially correlated with the electronic properties characterized by the *in-situ* photoluminescence measurements. The correlation reveals mesoscale structure-property relationship in TMDs. In the second example, we report the first femtosecond surface X-ray diffraction using the free-electron laser at Linac Coherent Light Source to quantify the ultrafast structural dynamics of monolayer WSe2 crystals supported on a substrate. We found the absorbed optical photon energy is preferably coupled to the in-plane lattice vibrations within one picosecond whereas the out-of-plane lattice vibration amplitude remains unchanged during the first ten picoseconds. The observed nonequilibrium anisotropic structural dynamics agrees with first-principles modeling in both real and momentum space, marking the distinct structural dynamics of monolayer crystals from their bulk counterparts.

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