

Thursday Afternoon, September 22, 2022

-Monteiro M. C. O., Schmuki P., Killian M.S. Metal-Phosphate Bilayers for Anatase Surface Modification. *Appl. Mater. Interfaces*. 2018, 10, 7, 6661-6672. doi.org/10.1021/acsami.7b16069

-Tombácz E. pH-dependent surface charging of metal oxides. *Per. Pol. Chem. Eng.* 2009, 53, 2, 77-86. doi: 10.3311/pp.ch.2009-2.08

Beyond SIMS

Room Great Lakes C - Session BS+SS-ThA4

Multi-Technique

Moderator: Andrew Giordani, Procter & Gamble Company

4:00pm **BS+SS-ThA4-13 In Operando Correlated Studies in Energy Materials via Combined Afm/ToF-Sims Platform, Anton V. Ievlev**, Oak Ridge National Laboratory, USA

The performance of energy storage and conversion devices, including batteries, fuel cells, and photovoltaics, is defined by the delicate interplay of electrical response and charge carrier migration at the nanoscale.

Although physical behavior and macroscopic functional response is well established, intrinsic chemical phenomena associated with ionic motion or localized electrochemical reactions can dramatically alter behavior and restrict utility of these materials. Over the last decade, advancements in development of novel characterization tools such as atomic force microscopy (AFM) have revolutionized our understanding of the electrical and mechanical response of materials; however, *dynamic* electrochemical behavior and ion migration remain poorly understood. Recently time-of-flight secondary ion mass spectrometry (ToF-SIMS) has proven to be effective tool for characterization of static chemical states in energy materials. However, its application to study of dynamic electrochemical processes still requires development.

Here we introduce approach based on combined AFM/ToF-SIMS platform for correlated studies of the dynamic chemical phenomena on the nanoscale in operando conditions. Being used for characterization of the perovskite materials it allowed direct observation of the ionic migration within the device in externally applied electric fields, which is important for fundamental understanding of the material functionality. Similarly, this approach allowed to study relaxation processes of the chemical phenomena in ferroelectric materials as a function of sample temperature. Altogether, developed approach enables direct characterization of interplay between chemical and functional response in energy materials and aids in the development and optimization of novel devices.

This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility and using instrumentation within ORNL's Materials Characterization Core provided by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy.

4:20pm **BS+SS-ThA4-15 Adsorption Differences of Organic Molecules on the Metal Oxide Surfaces, Aydan Yadigarli, S. Mohajernia, M. Killian**, Chemistry and Structure of new Materials, Siegen University, Germany; *M. Aktan*, Department of Materials Science and Engineering, KU Leuven, Belgium; *A. Braem*, Department Materials Science and Engineering, KU Leuven, Belgium

Tuning the surface properties of metal oxide allows to obtain an improved surface with new functionalities without compromising on the bulk properties of a substrate. Modification of oxide surfaces with self-assembled monolayer (SAM) has been introduced for advanced applications by changing the wettability, biocompatibility, adhesion, dye-sensitization, and chemical reactivity of the surface. The adsorption efficiency of SAMs on metal oxide surfaces depends on the molecular head group and inherent properties of metal oxide. Solution pH value influences the prevalent surface charging of metal oxides, which can be positive or negative depending on the isoelectric point (IEP) of the metal itself. Positively/negatively charged metal oxide surfaces lead to an attractive interaction with the negatively/positively charged functional head groups dissociated in the solution. In this study, the affinity of organic molecules with a selected range of specific head groups (carboxylic acid and amine) to metal oxides (TiO₂ and NiO) that are varying with their IEP was investigated. Compact metal oxides were formed by electrochemical anodization method and their IEP was found by zeta-potential measurement. Time of flight secondary ion mass spectrometry (ToF-SIMS) and X-ray Photoelectron spectroscopy (XPS) were used to confirm the chemically binding of the organic molecules. The coverage of the metal oxide surfaces was evaluated by contact angle measurement. The adsorption affinity of organic molecules has shown a relatable trend with the IEPs of the metal oxides.

References

Author Index

Bold page numbers indicate presenter

— A —

Aktan, M.: BS+SS-ThA4-15, 1

— B —

Braem, A.: BS+SS-ThA4-15, 1

— I —

Ievlev, A.: BS+SS-ThA4-13, **1**

— K —

Killian, M.: BS+SS-ThA4-15, 1

— M —

Mohajernia, S.: BS+SS-ThA4-15, 1

— Y —

Yadigarli, A.: BS+SS-ThA4-15, **1**