NORTHWESTERN UNIVERSITY'S DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING PRESENTS:

2021 MSE SPRING SEMINAR SERIES

Luis De Jesus, PhD

Provost Postdoctoral Fellow
University of Pennsylvania

Born and raised in Puerto Rico, Dr. Luis R. De Jesus obtained his B.S. in chemistry from the University of Puerto Rico at Cayey where he graduated with honors. From there, he joined Prof. Sarbajit Banerjee's research laboratory to pursue his Ph.D. at Texas A&M University where he focused on mapping electronic structure inhomogeneities and modeling spectroscopic signatures of electrode materials. During his graduate studies, Luis obtained a number of accolades, including the National Science Foundation Graduate Research Fellowship and the American Physical Society Robert S. Hyer Graduate Award. Additionally, he was awarded the IUPAC-Solvay International Award for Young Chemists, and the 2019 ACS-Division of Inorganic Chemistry Young Investigator Symposium Award given at the Fall ACS National Meeting in San Diego, CA. He is currently a Provost Postdoctoral Fellow working under the supervision of Prof. Thomas E. Mallouk at University of Pennsylvania. His current research interests involve the synthesis and functionalization of 2D layered MXene materials.

Comprehensive Nanoscale Evaluation of Electronic Structure Inhomogeneities in Layered Materials

The discovery and development of new materials tailored to a specific function remain as one of the grand challenges for materials' scientists. To this end, layered materials have been extensively studied due to the sundry of properties that emerge from chemical and physical modifications. Unfortunately, little is still known of the pronounced alterations to the electronic structure upon dimensional reduction to a two-dimensional (2D) structure or functionalization of their active sites. Comprehensive nanoscale characterization is essential to understand how the loss of 3D structural coherence and further modifications of the surface, induced as a result of ion intercalation, exfoliation to 2D sheets, or functionalization of the basal planes, alter the electronic structure of these materials which translates into physical properties. In this seminar, I will discuss the mechanisms of lithiation of layered α-V_2O_5 and the stark inhomogeneities to the crystal and electronic structure of this material during lithiation. X-ray microscopy observations indicate that the formation of lithiation gradients in individual nanowires of layered orthorhombic V_2O_5 arise from electron localization and local structural distortions. Electrons localized in the V_2O_5 framework couple to a local distortion, giving rise to small polarons. Additionally, increased inhomogeneity at the interfaces of a cluster of nanowires suggests an exchange of Li-ions, implying a "winner-takes-all" behaviour. Next, I will present the first direct visualization of patterns of compositional inhomogeneities within cathode materials during electrochemical discharge. Two distinct patterns are evidenced: core—shell separation and striping modulations of Li-rich and Li-poor domains within individual particles. In addition, 3D compositional maps have been developed and translated to stress and strain maps, providing a hitherto unprecedented direct visualization of stress and strain inhomogeneities. Finally, I will discuss my current work on the synthesis and structural modification of the canonical layered MXene: $Ti_3C_2T_x$. We show that the electronic structure of $Ti_3C_2T_x$ retains the carbide nature when using low concentrations of etchant, providing a synthetic route to increase the stability of these materials in water.

Thursday, May 13 • 4 PM CDT • Zoom

Registration is required. RSVP link.

Questions? Contact Kristina.lugo@northwestern.edu.

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