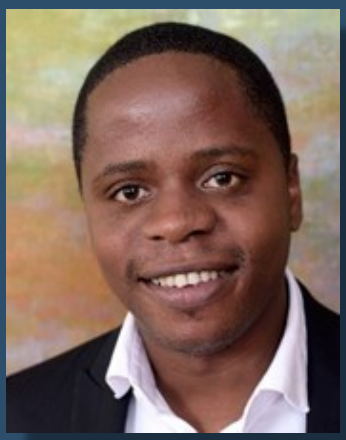
UNIVERSITY OF CALIFORNIA, IRVINE

Department of Materials Science and Engineering

Probing The Electronic States of Functional Materials From First Principles



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Zoom: **https://uci.zoom.us/j/97890617262?pwd=N3A1cXY3U0RkQjMwM0FGY1ZrUkd2QT09**

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Abstract: Determining the properties of the nanoscale region next to functional interfaces, relevant to electrochemical and electrocatalytic devices, is of fundamental importance, since symmetry breaking results in unique quantum mechanical effects, such as intermolecular charge transfer, as well as thermodynamic effects, such as frustrated entropy packing. These forces conspire to modify and complicate the interfacial structure and dynamics and represent a new frontier for nanoscale engineering and predictive design strategies aimed at improving device efficiency. In this talk, I will present our recent efforts aimed at obtaining quantitative information of the electronic states of nanoscale materials, under applied bias, using first principles based computer simulations and X-ray spectroscopy. Two model cases are presented: probing the surface structure and associated small molecule binding of polarized, ferroelectric thin films, relevant to the hydrogen evolution reaction, and probing the active states of transition-metal dichalcogenides during the electrochemical reduction of CO_2. We will also present an overview of our integrated theory/experiment training and professional development initiatives of students as part of the UC San Diego MRSEC.

Bio: Tod A Pascal is an assistant professor of NanoEngineering and Chemical Engineering at the University of California San Diego, and an affiliate faculty in the Material Science and Engineering program and the Halıcıoğlu Data Science Institute. He is a PI at the Sustainable Energy and Power Center and the UC San Diego MRSEC, co-leading a program on Predictive Assembly. Work in his research group focuses on advances theoritical and computational tools for studying phenomena at nanoscale interfaces, including those relevant for electrochemical devices and catalytic systems.