

SEMINAR

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Sala Montalcini

Defects in 2D Materials: What TEM Can, and Cannot, Show

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Host: Omar Ginoble Pandoli, Giorgio Divitini

Abstract

Missing sulfur atoms are thought to switch on the inert basal plane of MoS_2, turning it into an active catalyst for hydrogen evolution. Atomic-resolution electron microscopy should be the ideal tool to find them. So why is it so hard?
In this seminar, I will take a critical look at what (S)TEM can, and cannot, prove about defects in 2D materials, using defect-engineered MoS_2 as a test case. I will show how hydrocarbon contamination compromises atomic-resolution data and present the plasma-free protocol that consistently gave us clean lattices. Multislice simulations show that single sulfur defects drop below our detection limit in flakes only three layers thick, and that a sulfur vacancy and an oxygen substitution produce nearly indistinguishable contrast. Rather than stopping at what we cannot see, I will focus on what can be measured with confidence from images and diffraction: edges, terraces and pores, local phases and strain, and short-range order from electron pair distribution function (ePDF) analysis.
I will close with a new challenge we are starting with colleagues in Genoa: extending these lessons to sustainable, bamboo-derived electrodes modified with MoS_2. The talk is aimed at anyone who synthesizes, images or models 2D materials, and includes a brief introduction to the electron microscopy facilities at LNNano, part of CNPEM, the Brazilian research center that hosts the Sirius synchrotron.

Dr. Tarcísio M. Perfecto is a Technology Development Specialist in the Transmission Electron Microscopy Group at the Brazilian Nanotechnology National Laboratory (LNNano/CNPEM), where he is responsible for the double aberration-corrected Titan Cubed Themis. He holds a Ph.D. in Chemistry from São Paulo State University (UNESP) and was a FAPESP postdoctoral fellow at LNNano, working on transparent YAG ceramics. His research combines atomic-resolution (S)TEM, EDS and electron diffraction with Python-based workflows for large microscopy datasets, applied to 2D materials, functional nanomaterials, ceramics and gas sensors.