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Institut Català de Nanociència i Nanotecnologia

Manuel Cardona Lectures

These lectures provide the opportunity to hear from some of the most prominent researchers in nano-related fields.

They stand in tribute to **Prof. Manuel Cardona**, a key figure in the history of the ICN2.

Bits to Atoms and Atoms to Bits: Automated Experiment and Atomic Fabrication in Electron Microscopy

Sergei V. Kalinin

Department of Materials Science and Engineering
University of Tennessee, Knoxville, USA
sergei2@utk.edu

ABSTRACT

The last note left by Richard Feynman stated "*What I cannot create, I do not understand.*" Building solid state quantum computers, creating nanorobots, and designing new classes of biological molecules and catalysts alike requires the capability to manipulate and assemble matter atom by atom, probe the resulting structures, and connecting them to macroscopic world. In this presentation, I will discuss recent progress in automated experiment in electron microscopy, ranging from feature and physics discovery via active learning to direct atomic fabrication. I introduce the concept of the reward-driven experimental workflow planning and discuss how these workflows can be implemented via domain-specific hyper languages. The applications of classical deep learning methods in streaming image analysis are strongly affected by the out of distribution drift effects, and the approaches to minimize though are discussed. The real-time image analysis allows spectroscopic experiments at the predefined features of interest and atomic manipulation and modification with preset policies. I further illtrate ML methods for autonomous discovery, where the microstructural elements maximizing physical response of interest are discovered. These deep kernel learning (DKL) methods offer significant advantage compared to simple Gaussian Processes often tend to produce sub-optimal results due to the lack of prior knowledge and very simplified (via learned kernel function) representation of spatial complexity of the system. The DKL AE is illustrated via experimental discovery of the edge plasmons in STEM/EELS. The forensic analysis of the automated experiment makes the discovery process explainable and allows for human in the loop interventions. Finally, I will discuss the opportunities and strategies for direct atomic fabrication via electron beams, targeting desired structures and desired functionalities.

WEDNESDAY 8 MARCH AT 11:00 (CET)

ICN2 SEMINAR ROOM - https://icn2.cat/en/events

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BIOGRAPHY

Sergei Kalinin is a Weston Fulton Chair professor at the University of Tennessee, Knoxville. Prior to this, he has been corporate fellow and group leader at Oak Ridge National Laboratory (2002-2022) and principal scientist (special projects) at Amazon (2022-2023). He received his MS degree from Moscow State University in 1998 and Ph.D. from the University of Pennsylvania (with Dawn Bonnell) in 2002. His research focuses on the applications of machine learning and automated experiment methods in microscopy and materials synthesis and optimization, including physics discovery and atomic fabrication by scanning transmission electron microscopy, as well as mesoscopic studies of electrochemical, ferroelectric, and transport phenomena via scanning probe microscopy. Sergei has co-authored >650 publications, with a total citation of >47,000 and an h-index of >107. He is a fellow of MRS, APS, MSA, IoP, IEEE, Foresight Institute, and AVS; a recipient of the Feynman Prize of Foresight Institute (2022), Blavatnik Award for Physical Sciences (2018), RMS medal for Scanning Probe Microscopy (2015), Presidential Early Career Award for Scientists and Engineers (PECASE) (2009); Burton medal of Microscopy Society of America (2010); 4 R&D100 Awards (2008, 2010, 2016, and 2018); and a number of other distinctions.