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ARMS 1010

"Defects Are Not Statues: First-Principles Design Rules for Next-Generation Semiconductors"

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Abstract: Defects are not clerical details; they are the material. Over the past two decades, first-principles calculations based on density functional theory have turned that idea into a practical engine for semiconductor innovation: predicting which imperfections form, which charge they carry, how they interact, and how they ultimately control conductivity, recombination, and long-term stability. This seminar highlights the impact of this approach across a broad portfolio—II-VI photovoltaic absorbers (CdTe), III-nitrides (GaN, InN), transparent oxides (ZnO, In_2O_3), rutile TiO_2, and wide-band-gap perovskites ($SrTiO_3$, $KTaO_3$, $CaSnO_3$), and 2D materials. A recurring lesson is that defect physics is a coupled problem of thermodynamics and kinetics. Formation energies and charge-transition levels explain doping bottlenecks and compensation, identify likely recombination-active centers, and connect growth conditions to carrier densities. But many device-defining behaviors are kinetic: persistent photoconductivity and metastability under bias/illumination, defect–dopant complex formation that silently neutralizes intended doping, and carrier localization as small polarons that reshape transport and optical response. I will show how adding migration barriers—and, where relevant, polaron physics—can change the identity of the "dominant defect," reconcile seemingly contradictory experiments, and turn processing variables (chemical potentials, thermal budgets, quench rates) into quantitative levers for materials design.

Biography: Anderson Janotti is a professor in the Department of Materials Science and Engineering at the University of Delaware. He received his Ph.D. in Materials Physics from the University of São Paulo, Brazil, in 2000, where he carried out theoretical work on defects and surfaces of semiconductors. Following his Ph.D., he was a postdoctoral researcher at the National Renewable Energy Laboratory from 2000 to 2002, working on the computational design of novel photovoltaic materials for multi-junction solar cells, and then a Research Associate in the Metals and Ceramics Division at Oak Ridge National Laboratory from 2002 to 2004. In 2004 he joined the Materials Department at the University of California, Santa Barbara, as a Project Scientist, where he studied defects and doping in oxide and nitride semiconductors, complex oxides, high-κ dielectrics, and two-dimensional materials. He has been on the faculty at the University of Delaware since 2015, where his group uses first-principles electronic-structure methods and other computational tools to investigate defects, doping, interfaces, and novel materials for electronic and energy applications. Prof. Janotti has authored more than 250 research publications, with tens of thousands of citations and an h-index exceeding 85, reflecting broad impact in condensed matter and materials physics. He was elected a Fellow of the American Physical Society in 2016 by the Division of Materials Physics for his contributions to defect physics and doping in semiconductors, and he is a recipient of the NSF Faculty Early Career Development (CAREER) Award. He has been active in service to the materials physics community, serving on the editorial boards of materials and electronic-structure research journals.

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