

Physics Colloquium

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Unravelling the role of defects and small polarons in wide-band-gap oxide

Oxides are key materials for a wide range of applications, from (photo)catalysis to transparent conductors to memristors. In all these applications, intrinsic defects, impurities, and localization of charge carriers play major role in the materials properties and performance. Point defects such as oxygen vacancies have often been invoked to explain many of the interesting phenomena that are observed in oxides. Still, direct identification of point defects in these materials remains elusive, and proof of their existence has not been unambiguous. First-principles calculations based on the density functional theory have emerged as a powerful tool to study defects in crystals, and hybrid functional implementations have provided unprecedented accuracy in the description of point defects in semiconductors and insulators, and their impact on materials properties. These calculations often provide information that are difficult to access experimentally. In this presentation, we will discuss recent studies of point defects and impurities in prototype wide-band-gap oxides, such as ZnO, TiO₂, SrTiO₃ and CeO₂. We will draw comparisons and provide a broad picture of defect formation and stability in the different materials. We will also interpret some key experimental observations in the light of our first-principles calculations.



Dr. Janotti is an Assistant Professor in the Department of Materials Science and Engineering at the University of Delaware. He obtained his Ph.D. in Materials Physics from University of São Paulo, followed by a postdoctoral appointment at the National Renewable Energy Laboratory, CO, and a Research Associate position at Oak Ridge National Laboratory, TN. In 2004, he joined the Materials Department at the University of California Santa Barbara as a Project Scientist, and in 2015 he was appointed to the faculty at the University of Delaware.

Prof. Janotti's research covers computational design of novel materials for electronics and energy-related applications, with emphasis on processes involving defects, doping, interfaces and surfaces, using state of the art first-principles methods based on the density functional theory. He has published on a wide range of problems in materials physics, including novel photovoltaic materials for multi-junction solar cells, diffusion in high-temperature superalloys, defects and doping in oxides and nitrides, (de)hydrogenation processes in metal hydrides, nitride surfaces, high-k dielectrics, interfaces in complex oxides, and two dimensional layered materials. Prof. Janotti authored over 190 technical publications, with over 10,000 citations and an h-index of 54 in Google Scholar. He is a fellow of the American Physical Society.

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