



MATERIALS SCIENCE and ENGINEERING SEMINAR



Professor Gustav M. Dalpian

Institute of Physics

Santa Barbara University of São Paulo, Brazil

Trends in Artificial Intelligence for Materials Science: data generation, interpretability and property prediction

**MSEG
SEMINAR**
10/07/2026

04:00 p.m.

ISE 322

mseg.udel.edu

The integration of Machine Learning (ML) has transformed computational materials science far beyond simple property prediction. This seminar provides an overview of the diverse applications and current trends of ML in the field. We will explore key areas including the acceleration of materials discovery, challenges in robust data generation, and the deployment of open-source codes. The talk will also highlight advanced methodologies such as Natural Language Processing (NLP) for literature mining, graph-based representations for complex crystalline structures, and the critical need for interpretable ML models to ensure physical consistency. By examining these multifaceted computational strategies, we will demonstrate how artificial intelligence is fundamentally redefining modern research workflows in materials physics.

BIOGRAPHY

Gustavo M. Dalpian is a Full Professor at the Institute of Physics of the University of São Paulo (IFUSP), Brazil. He earned his Ph.D. in Physics from the University of São Paulo and completed postdoctoral research at the National Renewable Energy Laboratory (NREL) and at the University of Texas at Austin. His research focuses on computational condensed matter physics and materials modeling, specializing in electronic structure methods, machine learning applied to materials discovery, and the theoretical design of energy materials, including halide perovskites and two-dimensional systems.



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