講演会のご案内

このたび、メキシコ国立技術大学（TecNM）デュランゴ工科大学 電気電子工学科・大学院研究科のJosué Ortiz-Medina教授をお招きし、下記のとおり講演会を開催いたします。

Josué Ortiz-Medina教授は、グラフェンや二硫化モリブデン（MoS_2）などの二次元ナノ材料を対象とした電子特性解析や、人工知能（AI）を活用した材料シミュレーション分野で活躍されている研究者です。

本講演では、AIを用いて二次元ナノ材料の電子特性を効率的に予測する最新の研究成果についてご紹介いただきます。材料科学とAIの融合による新たな研究展開を学ぶ貴重な機会ですので、ぜひご参加ください。

【講師】

Dr. Josué Ortiz-Medina
Professor
Department of Electrical and Electronics Engineering,
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- **日　時：2026年 7月 16日（木）　13:30～14:30**
- **場　所：総合研究棟　1階 106室**
- **講演テーマ：2D Nanostructures Electronic Properties Prediction by AI: Tunneling the Ab Initio Mountain**

【講演概要】

グラフェンやMoS_2に代表される二次元ナノ材料は、優れた電子特性を有することから注目を集めています。一方で、その特性解析に用いられる第一原理計算には多大な計算コストが必要です。本講演では、人工知能（AI）の一種である深層畳み込みニューラルネットワーク（DCNN）を活用し、二次元ナノ材料の電子特性を高速かつ高精度に予測する最新の研究成果を紹介します。材料科学とAIの融合による新たな材料設計・解析手法の可能性について議論します。

主催：アクア・リジェネレーション機構　特別栄誉教授　遠藤守信

2D nanostructures electronic properties prediction by AI: tunneling the ab initio mountain

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The importance of 2D nanomaterials has been abundantly demonstrated during the last couple of decades, either from scientific research or technological developments points of view. Much of the early interest and research for this kind of materials was fueled by theoretical studies of fundamental nanostructures such as graphene and carbon nanotubes, which unveiled their remarkable electronic properties. The theoretical approaches used for the determination of such characteristics, usually termed as *ab initio* methods, are based on mathematical formulations of the Schrödinger equation, adapted to be computationally solvable. However, these methods are traditionally expensive, in terms of computational capacity and time requirements. It is here where the new computational methods related with *Artificial Intelligence* (AI) represent an interesting alternative to conventional ab initio approaches. This lecture explains recent results on the use of particular types of AI models, termed Deep Convolutional Neural Networks (DCNNs), which are algorithms of Machine Learning subclass. These methods have been explored recently to predict Scanning Tunneling Microscopy (STM) images of doped and/or defective graphene nanoparticles, based on ab initio simulations. Also, DCNNs models have been applied to the prediction of the spatial distribution of electronic wavefunctions, which are commonly used to project the volumetric representation of atomic or molecular orbitals. The results demonstrate that the use of AI models for the analysis of electronic properties of 2D nanostructures as the ones studied, which include graphene and a MoS_2 model, would allow for quick and efficient computational simulations/determination of electronic properties of 2D nanostructures. The discussed research contributes to implement and assess the impressive expansion of AI methods towards many science and technology areas, including materials science and nanotechnology.