[Energy Distinguished Lecture Series]

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Explainable AI for Correlative Spectroscopic Analysis of Low-Dimensional Materials

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Abstract

Low-dimensional materials exhibit highly heterogeneous optical and electronic properties that are strongly influenced by local variations in strain, doping, defects, and dielectric environment. Correlative spectroscopic and microscopic measurements provide complementary information on these spatially varying properties, but extracting physically meaningful relationships from high-dimensional multimodal datasets remains challenging. Here, we present an explainable artificial intelligence (XAI) framework for the correlative analysis of spectroscopic and microscopic data from low-dimensional materials. Machine learning models are employed to identify nonlinear relationships among spatially resolved optical, structural, and electronic observables, while XAI methods are used to determine which spectral features and local parameters contribute most strongly to the model predictions. By combining data-driven analysis with physical interpretation, the framework enables the identification of characteristic spectral signatures associated with variations in local material properties. The extracted relationships are further examined in conjunction with first-principles calculations to connect experimentally observed correlations with their microscopic origins. This approach demonstrates how XAI can move beyond conventional prediction tasks and serve as a tool for discovering physically interpretable relationships within complex correlative measurements. The proposed framework provides a general strategy for integrating multimodal spectroscopy, artificial intelligence, and computational modeling toward a more comprehensive understanding of heterogeneous phenomena in low-dimensional materials.

Brief Bio



Jaekak Yoo is an Assistant Professor at Hanyang University, Seoul, Korea. His research focuses on artificial intelligence-assisted spectroscopy, explainable AI, and computational modeling for low-dimensional and semiconductor materials. He received his Ph.D. in Energy Science from Sungkyunkwan University, where he investigated correlative optical spectroscopy of two-dimensional nanomaterials using machine learning, explainable AI, and first-principles calculations. After completing his Ph.D., he conducted postdoctoral research at Hanyang University, followed by postdoctoral research at the University of Illinois Urbana-Champaign, where he worked on AI-assisted spectroscopic imaging and computational nanophotonics. His current research aims to integrate multimodal spectroscopy, machine learning, and physics-based modeling to uncover interpretable structure-property relationships in advanced materials.

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