2024년도 대한전자공학회

하계종합학술대회 초청강연 발표준보

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▌초청강연 정보

제 목	Analyzing Molecular Structures with Graph Neural Networks
Abstract	This talk introduces and discusses the role of Graph Neural Networks (GNNs) in molecular structure analysis in computational chemistry and biology. Our focus will be on the adaptation and optimization of GNN models designed to handle the complexity of structures of molecules, proteins, etc. These models are particularly adept at capturing the topological and feature-based relationships inherent in molecular graphs, facilitating interpretation and robust prediction. We present a systematic overview of the latest methodologies in GNNs, including novel training techniques and model designs that improve model interpretability and prediction performance. In addition, case studies will be discussed to demonstrate the practical applications of these models. This presentation aims to provide a comprehensive perspective on the current state and future prospects of GNNs, underscoring their critical contribution to accelerating drug discovery and material innovation through sophisticated AI-driven analysis.