Molecular Hypergraph Neural Network

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Graph neural networks (GNNs) have exhibited promising performance on many chemistry-related tasks. However, ordinary graphs only model the pairwise connectivities in molecules, can’t adequately describe higher-order connectivities like multi-center bonds and conjugated bonds. To address this challenge, we introduce molecular hypergraphs and propose Molecular Hypergraph Neural Network (MHNN) to predict the optoelectronic properties of organic semiconductors. MHNN outperforms all baseline models on the most tasks of organic photovoltaic (OPV) dataset. Without any 3D geometric information, MHNN also surpasses the baseline models using atom positions. Moreover, MHNN achieves better performance than pretrained GNNs under limited training data, demonstrating its excellent data efficiency.