Deep Graph Learning for Corrosion Inhibitor Performance Prediction and Optimization

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Abstract Corrosion is the primary cause of material degradation in industrial applications[1]. The application of corrosion inhibitors [2] is essential in preventing and mitigating the corrosion of metal components. Nevertheless, to select and design corrosion inhibitors suitable for specific materials and environments, researchers often rely on time-consuming laboratory experiments and gradually modify the structures of existing inhibitors[3]. Material chemists expect to identify the critical chemical substructures that affect corrosion inhibition performance to gain actionable insights, such as hints for inhibitors' structural optimization.

With the rapid development of artificial intelligence (AI) technology, deep learning models have attracted attention for their exceptional feature extraction and representation capabilities, particularly in domains involving graph-structured data[4]. Molecules, composed of atoms connected by chemical bonds, can be naturally represented as graphs, with atoms as nodes and bonds as edges[5]. The integration of deep graph learning into materials science may expedite the process of selecting and designing corrosion inhibitors. This study proposes a graph interpretation-based substructure mining method and constructs a graph neural network (GNN) model [6] to predict the inhibition efficiency (IE) of molecules. Fig.1 illustrates the overall framework of our model. Our model integrates multi-scale features and identifies critical substructures that significantly impact IEs. The model highlights the chemical substructures responsible for high IEs and provides a chemistry-intuitive explanation of structure-property relationships, facilitating rapid and precise IE predictions.

The results demonstrate that GNN-based models outperform traditional machine learning methods in prediction accuracy and computational efficiency, with a 7% RMSE. The models are poised to become reliable tools for selecting and optimizing

inhibitors. Compared to traditional methods that rely on intuition or experience, the data-driven graph interpretation method assists chemists in identifying chemical substructures with corrosion inhibition properties, guiding the design of effective new corrosion inhibitors.

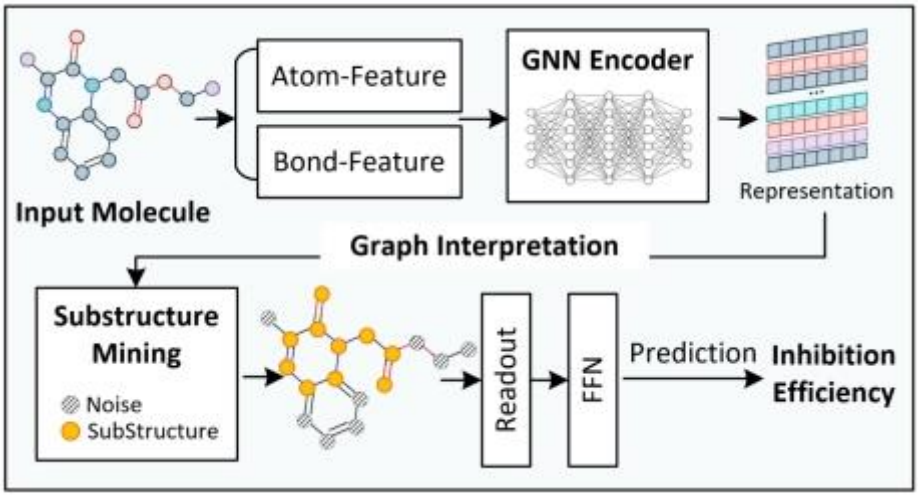

Fig.1 Overall Framework of IE Prediction Model based on Substructure Mining.

Keywords Corrosion Inhibitor, Deep Graph Learning, Substructure Mining, Graph Interpretation, Property Prediction

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