Simulation of Nanosystems for Energy Conversion
Department of Electrical and Computer Engineering
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Prediction of charge mobility in organic semiconductors using deep learning

Motivation

Organic semiconductors are rapidly finding applications as active materials in a large number of electronic devices such as light-emitting diodes, organic solar cells, field-effect transistors, and switches. However, their low charge mobility remains a bottleneck in their widespread and commercial applications. Computational modelling can play a major role in identifying the key microscopic parameters determining the carrier mobility and consequently developing *in silico* design strategies for organic materials with improved transport properties. Recently machine learning methods, especially deep learning, demonstrated impressive performance in predicting material properties based on molecular and structural attributes. Its extension to predict charge mobility in organic semiconductor remains a promisingly unexplored area.

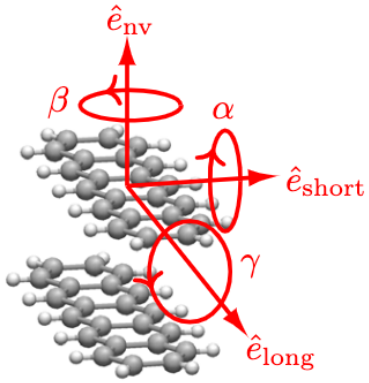

Figure 1: Prediction of transfer integrals between pentacene molecules.[1]

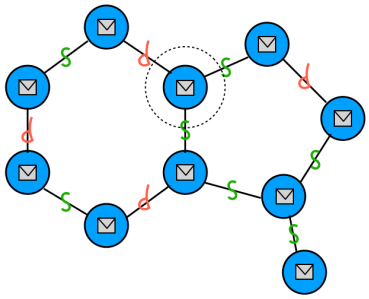

Figure 2: Message passing graph neural network

During the last few years, graph neural network has emerged as a suitable, robust and powerful machine learning model for representing molecules and predict material properties. Graph networks are natural choices for molecules since it can represent any molecule with any arbitrary connectivity.

Goals

The goal is to apply graph neural network for predicting charge mobility in organic semiconductors. Once the deep learning architecture is developed, it will be extended from small organic molecules to polymers. Application of transfer learning and coarse graining will be explored.

Requirements

- Knowledge in deep learning and interest in organic semiconductors
- Programming skills

Duration This topic is suitable for Masters thesis (6-12 month).

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1. Jonas Lederer, Waldemar Kaiser, Alessandro Mattoni, and Alessio Gagliard *Adv. Theory. Simul., 2, 1800136* (2019)