Development of a quantum chemical methodology in combination with machine learning for the theoretical design of functional polymers

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（機能性高分子の理論設計のための機械学習と組み合わせた量子化学的手法の開発）

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論 文 内 容 の 要 旨

Thesis Summary

Due to the rapid advancement of computational hardware and software as well as theoretical methodologies, quantum chemistry has become a powerful tool in polymer science for the prediction, design, and study of polymers. This thesis contributes to the development of quantum chemical methods in combination with machine learning towards computational investigation of functional polymers. The applications of developed methods include industrial push-pull organic polymers with nonlinear optical properties and the biopolymers such as DNA.

The first part of the work is devoted to the investigation of electronic structure and nonlinear optical (NLO) response in the [2.2]paracyclophane-containing polyphenylene vinylene polymers. The NLO response in these polymers can be controlled by alternation of donor and acceptor terminal substituents and extension of π-conjugated molecule linker. The original Elongation (ELG) method in combination with machine learning (ML) were used to investigate the effect of various donor/acceptor pairs and molecule length on the NLO response of these polymers under the external electric field. The produced data was utilized to train deep Neural Network (NN) to accurately predict a molecular hyperpolarizability of the analogous polymers. In order to get a valuable chemical insight, several ML interpretation techniques were used to uncover the relationships between input molecule descriptors and output target property learned by the NN.

The second part of the work devoted to the transition mutation from the Cytosine⋯Guanine base pair to the Adenine⋯Thymine base pair in DNA caused by the O^6-methylguanine lesion. In order to estimate the stability of the base pairs and understand the driving force of mutation, the original Through-space/Through-bond (TS/TB) orbital interaction analysis was programmed and utilized. Using TS/TB analysis, single intra- and inter-base chemical bond energies were calculated via cutting off the target orbital interactions. The main findings supported the experimental data about the relative stabilities of the base pairs in DNA duplex, while the geometry alignments of the mutation site were confirmed to be the main reason of mutation.