Green innovation, Energy production, Materials informatics

Development of next-generation solar cell by combining experiments and data science

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Abstract

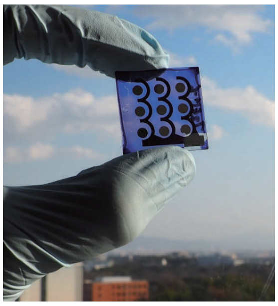
High-efficiency, low-cost next-generation solar cells have been developed as a sustainable energy source, and organic solar cells that do not contain toxic elements are one of the most plausible candidates. In this research, we perform a high throughput exploration of solar cell materials by combining a unique evaluation method based on microwave spectroscopy and machine learning. Organic-inorganic hybrid materials such as perovskite solar cells are other materials of target.

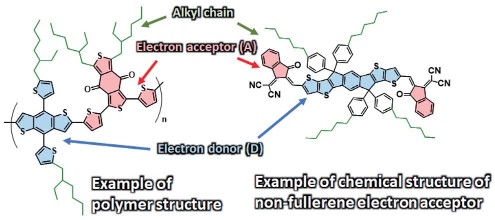
Background & Results

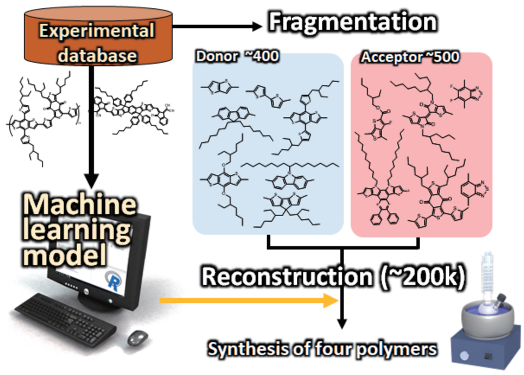
Compared to commercially-available inorganic solar cells such as silicon, organic solar cells are expected to be used on building walls, owing to the light weight and low cost production. However, there are infinite chemical structures of organic materials, and therefore it takes a lot of time and effort to design, synthesize, and evaluate new materials. In this research, we focus on polymer solar cells consisting of polymers and non-fullerene electron acceptors, which is designed by a machine learning model based on experimental data. A high throughput screening of polymer materials revealed the top-ranked new polymers, which were actually synthesized and characterized. The experimental results of the solar cells showed a good agreement with the machine learning prediction. Accordingly, we have succeeded in demonstrating the effectiveness of material development, which opens up a new avenue to the development of more efficient polymer solar cells and the research that integrates experiments and machine learning in materials science.

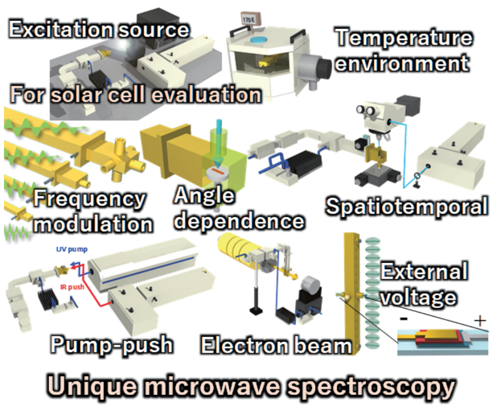
Significance of the research and Future perspective

In this research, we have developed an efficient experimental screening method using a unique microwave spectroscopy and a machine learning model to explore polymer materials for organic solar cells at a very high speed. We constructed a machine learning model using polymer and non-fullerene solar cells and screened virtually generated 200,000 types of polymers. Based on this result, a new polymer was synthesized and compared with the predicted value of machine learning, and a good agreement was obtained. In particular, the machine learning model was able to predict the structure of the optimum alkyl chain shape and length for the specific polymer backbone. The high-precision machine learning model demonstrated in this research can be a powerful tool for future polymer solar cell development.









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