

# Analysis of Molecular Aggregation in Organic Amorphous Devices

## 有機非晶デバイスにおける分子凝集構造解析

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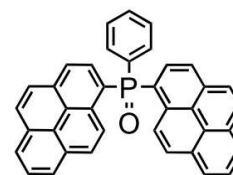
Tremendous kinds of organic molecules have been synthesized, aiming for organic devices with excellent performances. In addition to the synthesis of such various kinds of molecules, the analysis and control of the conformations and aggregated structures, such as molecular orientations, are also considered to be important, because they have significant impacts on the device performances. However, the conformations and aggregated structures have not been well analyzed yet, because organic molecules in devices are often in amorphous states and the precise analysis has been difficult. Under such circumstances, we have recently started solid-state NMR analysis, which enable us to analyze the conformations and aggregated structures in detail even for the materials in amorphous states.

In this study, first, we investigate the relationship between the device performance and device fabrication process, the deposition rate, for a phosphine oxide material (POPy<sub>2</sub>, Fig 1), which has an excellent electron-transport property. From the experiments on POPy<sub>2</sub> deposited films with the deposition rates of 0.1, 1.0, and 4.0 nm/s, we found that the carrier mobility became higher with increasing the deposition rate. The materials used in the devices are the same; therefore, the increase of the mobility is considered to originate from the different intra- or inter-molecular structure of POPy<sub>2</sub> in the deposited films. To reveal the structures and finally to understand the mobility change, we carried out <sup>31</sup>P chemical shift anisotropy (CSA) measurements in solid-state NMR. The P=O direction in POPy<sub>2</sub> molecules relative to the substrate can be monitored by the <sup>31</sup>P CSA measurements. From the experimental CSA spectra, it was found that POPy<sub>2</sub> molecules were not in completely random orientation but in an oriented state where the P=O directions were tend to orient perpendicular to the substrate, even for the lowest deposition rate in this study, 0.1 nm/s. With further increase of the deposition rate, higher orientation was found.

The molecular orientation in the thin films revealed by solid-state NMR is considered to be the origin of the improvement of the carrier mobility. To confirm the structure-property relationship, further solid-state NMR experiments and quantum chemical calculations have been in progress in our laboratory.

Recently, high-speed vacuum-deposition of organic molecules is attempted to attain cost-effective device fabrications, but the high-speed deposition often impairs the device performance. The above results show that both the improvement of device performances and the lowering of device fabrication cost can be achieved simultaneously, which is important for the commercial aspect of organic devices.

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**Fig. 1.** Chemical structure of POPy<sub>2</sub>.