**Functions of Molecular Arrangement**

Polymorphism, a phenomenon that a single molecule crystallizes differently, has an impact on the materials’ function, hence it is associated with pharmaceutics, food science, dyes and pigments, and organic electronics. We are working on crystal engineering problems through experimental and theoretical approaches.

Our original microscope absorption spectroscopic system enabled us to distinguish the photo-/thermal response at a single crystal level, to clarify their properties dependent on crystalline polymorphs (Cryst. Growth Des. 2019).

With combined quantum chemical and classical mechanics methods, we calculate the energy profiles of molecules, to clarify the crystal structure-molecular dynamics relations.