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Resolving terahertz spectral mixtures using the blind source separation approach: A method to study the dehydration kinetics

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Terahertz spectroscopy has gained popularity as a promising non-invasive investigation tool in recent decades. In studies of solid-state pharmaceuticals, its usefulness is enhanced, since it enables one to distinguish different polymorphic and pseudo-polymorphic forms. Terahertz absorption spectra are additive, meaning that the resulting spectrum of two or more compounds in the sample is an algebraic sum, in the linear region of the Beer's law. For this reason, the evolving-in-time linear mixture of unknown pure components can be resolved using the blind source separation approach, where both spectral sources and their concentrations are to be estimated. Such an evolution occurs naturally in temperature-induced (pseudo) polymorphic transitions, i.e. dehydration, where the terahertz spectrum is the hydrate and dehydrates's response with time-varying proportions. Conventionally, to estimate the kinetics of a reaction–an important physical-chemical parameter–the area of the unique spectral peak is integrated and normalized to evaluate the abundance, but a difficulty of strongly overlapping peaks unable its application. To overcome this problem, we show, that by employing the blind source separation procedure, we can resolve a complex, multi-compound spectral mixture with significant cross-bands, where the peak area method failed. We evaluate the performance of our approach in studies on dehydration of a well-known polycrystalline hydrate–α-D-glucose monohydrate. Seeing that the polymorphic transitions can completely change the properties of a pharmaceutical, our approach can find application in a drug development process, where their careful characterization is of utmost importance.

Biography

Lukasz A Sterczewski has received his MSc degree in Electronics from Wroclaw University of Technology, Poland in 2014, working on terahertz time-domain spectroscopy. He is currently working towards a PhD degree from WrUT. In September 2015 he has joined PULSE (Princeton University Laser Sensing Laboratory) as a Visiting Student Research Collaborator. His research is focused on development on new spectroscopic techniques and advanced signal processing tools.

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