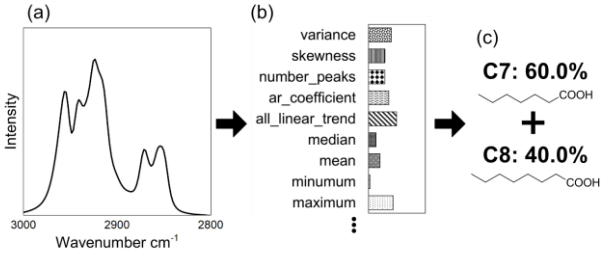
In-situ Compositional Identification of Mixed Aliphatic Molecules Adsorbed on Metal Oxide Nanostructures via Machine Learning of Infrared Spectrum

([1]*Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo*, [2]*JST-PRESTO,* [3]*Institute of Materials Chemistry and Engineering, Kyushu University*) ○Wenjin Lei[1], Chaiyanut Jirayupat[1], Takuro Hosomi[1,2], Kazuki Nagashima[1,2], Tsunaki Takahashi[1,2], Wataru Tanaka[1], Takeshi Yanagida[1,3]

Keywords: FT-IR; VOC; Machine Learning; Metal Oxide

Extracting *in-situ* composition values of molecular mixtures on surfaces of metal oxide nanostructure is clearly important for various chemical research fields including heterogeneous catalysts and molecular sensors, but still a challenging issue especially for similarly shaped molecules. Recently, machine learning technique was combined with various spectroscopy methods to quantify existing components.[1, 2] Here we propose a rational methodology for in-situ compositional identification of mixed similar aliphatic molecules adsorbed on metal oxide surfaces via machine learning of infrared spectra. This method analyzes FTIR spectra characteristic shapes of CH_2 and CH_3 vibration band (2800-3000 cm^{-1}), which appears on every FTIR spectra of VOCs, by machine learning algorithm with automatically extracted spectral features. Although these FTIR spectra wavenumbers are insensitive to the carbon number of aliphatic chains, the spectra shapes and relative intensity between different vibration bands are rather sensitive even for the one-carbon difference in aliphatic chains due to the coupled vibration nature throughout molecules.

We attempted to build machine learning models with FTIR spectra of 24 mixtures of 3 carboxylic acids (C7-C9). Then, they were applied to identify the composition ratio of molecules on ZnO nanowire surface. These results corresponded to those obtained through gas chromatography. Thus, the proposed method successfully discriminated the composition ratio of mixed aliphatic carboxyl acids with different carbon numbers. This method offers a useful approach to identifying *in-situ* compositions of various mixed aliphatic molecules on metal oxide surfaces. In this presentation, we will report further results and information, including the applicability of this method for various functional groups, such as aldehydes, alcohols, and amines.



(a) FTIR spectrum of C7/C8 acid mixture on ZnO surface, (b) Extracted features (>400), (c) Prediction

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