Moving Past Phase Sensitive Detection in Modulation Excitation Spectroscopy

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SEMINAIRE

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Modulation Excitation Spectroscopy associated to Phase Sensitive Detection (MES-PSD) allows selectively detecting and identifying intermediates involved in reversible reactions, and is now being used more and more to characterize heterogeneous catalytic processes. In this lecture, the basis of Phase-Sensitive Detection (PSD) will be revisited to highlight its limitations and to introduce alternative workflows for analysing ME spectra directly in the time domain.
It will be shown that PSD effectively performs a linear transformation of averaged difference spectra, efficiently suppressing noise but at the cost of reducing information on reaction profiles. In particular they exhibit much stronger correlations in the phase domain than in the time domain. This (i) hinders the detection of transient intermediates and (ii) reduces the ability to discriminate between concurrent reactions. These effects are demonstrated through both simulations of model systems and analyses of recent open-source, and in-house experimental datasets.

Two complementary multivariate workflows will be introduced for analyzing ME spectra directly in the time domain. The first, MES-DAS (Denoise–Average–Subtract), incorporates a multivariate denoising step prior to the averaging and subtraction operations, yielding time-domain difference spectra with significantly reduced noise. The second, MES-CP (Candecomp/Parafac decomposition), factorizes the full three-way tensor of non-averaged spectra to recover spectral and kinetic profiles directly. Both approaches achieve noise-reduction performance comparable to PSD while preserving the resolution of kinetic profiles. Notably, MES-CP also removes the strict reversibility constraints inherent to PSD, making it particularly well suited for systems involving irreversible phenomena such as surface accumulation or catalyst deactivation.

Formalités d'entrée : accès libre dans l'amphi du pavillon d'Accueil.
Si la manifestation a lieu dans le Grand Amphi SOLEIL du Bâtiment Central merci de vous munir d'une piece d'identité (à échanger à l'accueil contre un badge d'accès).

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