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Raman to monitor changing materials and materials in change

Raman is uniquely suited for the real-time monitoring of both dynamic chemical processes (“changing materials”) and structural transformations (“materials in change”) across catalytic, material, and biological systems [1, 2]. First, in industrial reaction monitoring, real-time in situ Raman spectroscopy tracks the solvent-free liquid-phase epoxidation of cyclohexene with tert-butyl hydroperoxide over alumina-supported vanadium and phosphorus oxide (VPO) catalysts, following reactant depletion (C=C stretching at 1654 cm^{-1}) and product formation (1,2-epoxycyclohexane C-O-C modes at 784 cm^{-1}) [3]. The emergence of two distinct isosbestic points (at 841 and 832 cm^{-1}) confirms a direct reaction pathway without stable intermediates [3]. If a reaction does have stable intermediates, the isosbestic point won’t be present [4]. Second, this inline monitoring paradigm is applied to zeolite hydrothermal crystallization, specifically tracking the interzeolite conversion (IZC) of metastable faujasite (FAU) to stable gismondine (GIS) [4]. Non-negative least squares (NNLS) deconvolution of solid-phase in situ Raman spectra (450–530 cm^{-1}) yields quantitative phase fractions that strongly correlate with ex situ X-ray diffraction (XRD) Rietveld refinements [5]. Third, we explore the biophysical interplay of environmental plastics, analyzing how microplastics biotransform inside the human gastrointestinal tract and interact with the colonic microbiota (simgi® simulator) [6,7]. Finally, strategies for spectra acquisition and to transition these diverse applications from isolated solutions to scalable automated workflows stand on data harmonization [1]. Fostering an open and FAIR (Findable, Accessible, Interoperable, and Reusable) ecosystem, adopting standardized hierarchical data structures (NeXus/HDF5, NXraman) [1,5], domain-specific ontologies (Vibrational Spectroscopy Ontology – VIBSO), traceable calibration protocols (CWA 18133/18134) [1], and database federation [1]. Aligning spectroscopic practices with FAIR principles represents a paradigm shift that will unleash the full potential of artificial intelligence (AI) and chemometrics across academic and industrial manufacturing [1].

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