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Operando Raman methodology, getting a grip on structure-performance of working functional materials: the catalysis instance

Understanding functional materials at a molecular level is connecting its performance with the structure it has during operation. The concept behind *operando* methodology is that the functional material must be characterized while working in an array that allows simultaneously measuring its performance free of distortions imposed spectroscopic cell features. The working condition of some functional materials are of different nature; touching base in the case of catalysis, this requires reinventing the spectroscopic cell from a cell where you mimic reaction conditions. This is a generalized change of gears in catalysis science [1]. Since it was first proposed in literature in 2002, with three papers [2][3][4], there has been an exponential growth on its use with more than 1070 papers in 2023 (Scopus). An *in situ* study will report on the state of the catalyst while working but will fail to report what is the real catalytic performance. The operando methodology for catalysis requires taking spectroscopy to the catalytic reactor rather than bringing the catalytic reaction to an *in situ* cell. We will present how *operando* reactors are and show Raman *operando* instances that simultaneously report changes in the catalyst structure/surface species and on its performance.

Along with experimental rigs, *operando* Raman methodology need detailed spectral analyses and may in turn be used for process control. Hence, within CHARISMA project, we are working not only on harmonization of Raman spectra, but also on adapted data formats that include all process and processing metadata. These approaches are relevant for research made in other applications.

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