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**From molecules to materials and from materials to molecules:
a fantastic playground seen by the eye of a spectroscopist**

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Multi technique approaches, combined with molecular modelling will be used to describe the evolution of molecular species and materials, aiming to disclose their properties when they act as catalysts. Few examples will be selected as case studies to show crucial points in the investigation of these species through in situ spectroscopies. The contribution will try to describe what are the strengths and weaknesses of some of the most used techniques in understanding the local structure of the active site and what is the role of molecular modeling in supporting the understanding of the system under consideration. Moreover, the contribution will try to consider how it is possible to perform a structure-catalytic properties correlation to develop new catalysts with better performances.

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