Ultrafast electron dynamics of metallic/metal oxide nanostructures in relation to environmental catalysis

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ABSTRACT

This project aims at gaining scientific insight on how fundamental electronic processes at the microcosmos of metal/metal-oxide nanostructures are influencing the catalytic properties of nanoparticle-based catalysts in the model catalytic oxidation of CO and VOCs.

The synthesis parameters of the nanoparticles control their structural and optical characteristics. They will be grown using the method of citric acid complexation in possible combination with hydrothermal treatment or alternatively with evaporation/sputtering techniques. Their growth parameters are in turn expected to strongly influence the ultrafast electronic interactions of the resulting nanostructures. These will be studied by time-resolved laser spectroscopy. This method is chosen due to its unique ability to investigate the very short timescales (10^{-15}-10^{-12}s) in which ultrafast electronic interactions take place. Transition metal oxides have been rarely examined, typical examples being the study of oxygen vacancies in tungsten oxide samples and the photoreduction of δ-MnO_2.[1,2] Also, only one report exists on the ultrafast dynamics during in situ catalytic oxidation of CO by metal oxide catalysts.[3] Finally, the catalytic performance will be studied using the oxidation of CO and VOCs as probe reactions.

Thus, we will employ complementary techniques in order to interrogate both the microscopic (ultrafast electron dynamics) and the macroscopic (catalytic performance) properties of the grown systems. In this way, we expect to acquire a deeper and spherical understanding of the physics leading to the catalytic properties of metal/metal-oxide nanostructures and explore the optimal conditions to control and enhance their catalytic properties. If the progress of the proposed project allows for it, we will extend our research to the in-situ study of the ultrafast domain of the catalytic process in the model CO oxidation case.

Successful execution of the project will bring environment-friendly solutions to societal problems, such as air quality, production of renewable/sustainable fuels and environmental protection (emissions control, water quality), that are in the forefront of the funding policy of the EC. Also, young scientists will be trained in hot research areas and will therefore gain a boost in their competencies to stand up in up-to-date scientific challenges.

Preliminary results and comments are hereby presented.

REFERENCES

[1] Zhang, X. P. *et al.* Femtosecond visualization of oxygen vacancies in metal oxides. *Sci Adv* **6**, doi:ARTN eaax9427.
[2] Marafatto, F. F. et al. Rate and mechanism of the photoreduction of birnessite (MnO_2) nanosheets. P Natl Acad Sci USA 112, 4600-4605, doi:10.1073/pnas.1421018112 (2015).
[3] Wagstaffe, M. et al. Ultrafast Real-Time Dynamics of CO Oxidation over an Oxide Photocatalyst. Acs Catal 10, 13650-13658, doi:10.1021/acscatal.0c04098 (2020).