NewTimes – New Trends in Materials Science and Engineering
1st International Virtual Conference
14-18 June 2021

SESSION: *Advanced materials for water treatment and environmental protection*
Preference: ORAL presentation

Origin of Visible Light Photo-degradation ability of the CeO_2/ZnO Heterojunction

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In 2019 the World Health Organization has reported that more than 10.000 people die every day for the onset of diseases related to water contamination. [1] In this regard, to the concentration increase of the so called *Persistent Organic Pollutants* (POPs), an increment of the emergent pollutants (CECs, *Contaminants of Emerging Concern*) arising from the development of the welfare society has been recently recorded. In this background, the growing interest of the scientific community in the area of heterogeneous photocatalysis is legitimized by the mandatory requirement to reduce the water contamination caused by human activities. Indeed, heterogeneous photocatalysis is one of the most promising *Advanced Oxidation Processes* (AOPs) allowing the complete photo-degradation of classical and emerging harmful pollutants in wastewater.
Among the tested materials, nanostructured transition metal oxide semiconductors have been identified being the most suitable for photocatalytic applications. This feature arouses from their intrinsic band structure allowing them to induce the promotion of electrons into the conduction band – CB, leaving holes in the valence band – VB, when an appropriate amount of light energy (UV – visible light), is applied. Once at the semiconductor surface, the photo-generated charge carriers can facilitate reductive and oxidative redox reactions, respectively; these lead to photo-oxidation processes inducing the complete mineralization of the pollutants. Unfortunately, the fraction of charge carriers really available in a photocatalytic process is very poor, since the most probable process is the electron–hole pair recombination, limiting the amount of free electrons and holes for redox reactions. For this reason, the development of new photo-active materials is essential and highly required in order to overcome this drawback.
In this contribution we show the photocatalytic ability of the CeO_2-ZnO mixed system upon visible irradiation ($\lambda \geq 420$ nm) in the photo-degradation of a persistent emerging contaminant as Acesulfame-K. In particular, we focused on the structural, optical and electronic characterization of the biphasic solid, highlighting the role of the oxide interfaces. Especially with an EPR-based approach, we were able to monitor and quantify the charge separation processes at the materials interface and at their surfaces. Finally, DFT calculations provide a rational for the observed phenomena on the basis of a band alignment of the two systems as a consequence of the formation of a heterojunction, justifying the occurrence of a visible-light activity thanks to the presence of the empty localized Ce^{4+} *4f* orbitals. [2]

[1] WHO & UNICEF. Progress on household drinking water, sanitation and hygiene 2000- 2017. Special focus on inequalities. (United Nations Children's Fund and World Health Organization, 2019).
[2] E. Cerrato et al. ACS Appl. Energy Mat., 1 (2018) 4247-4260.

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