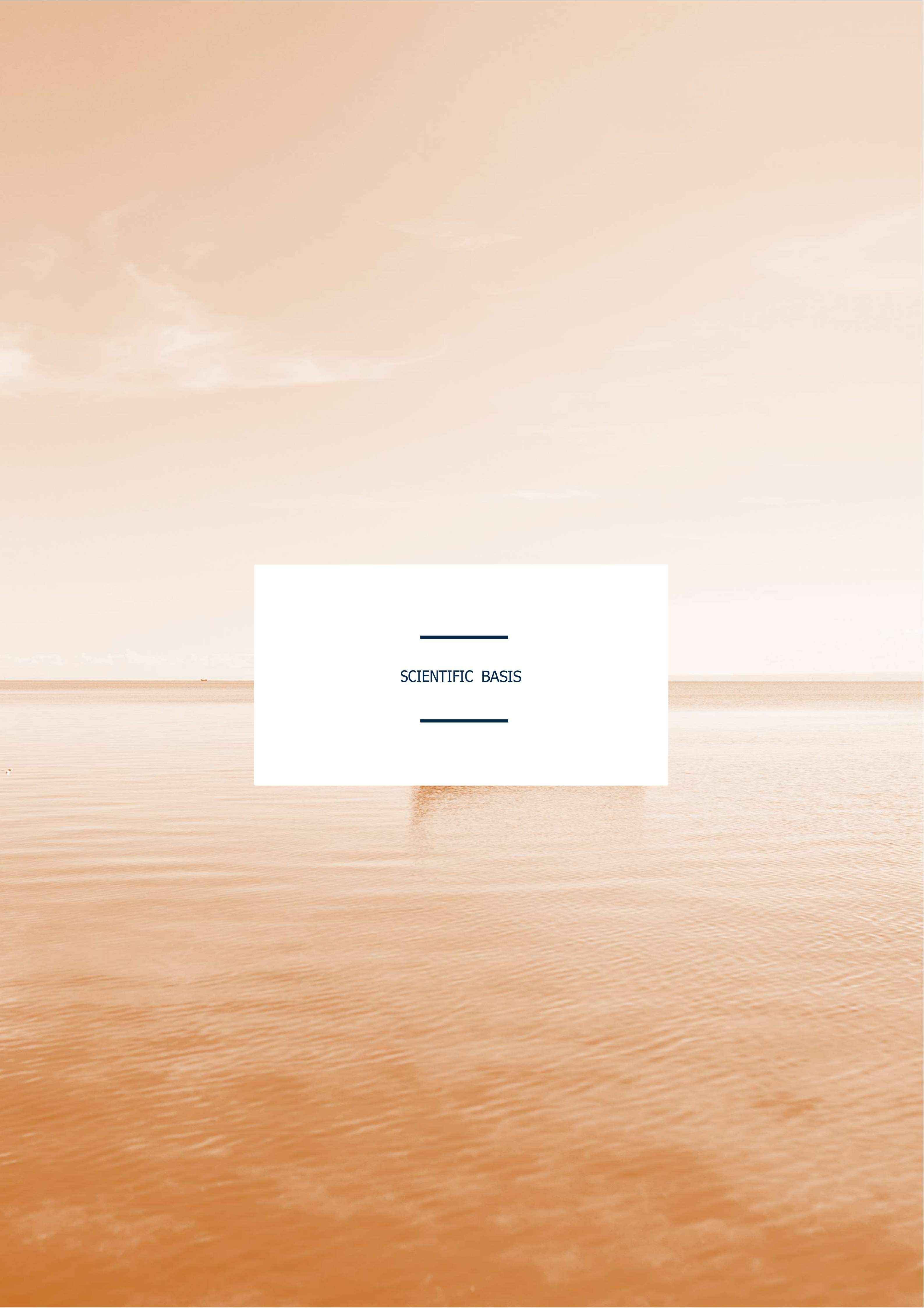
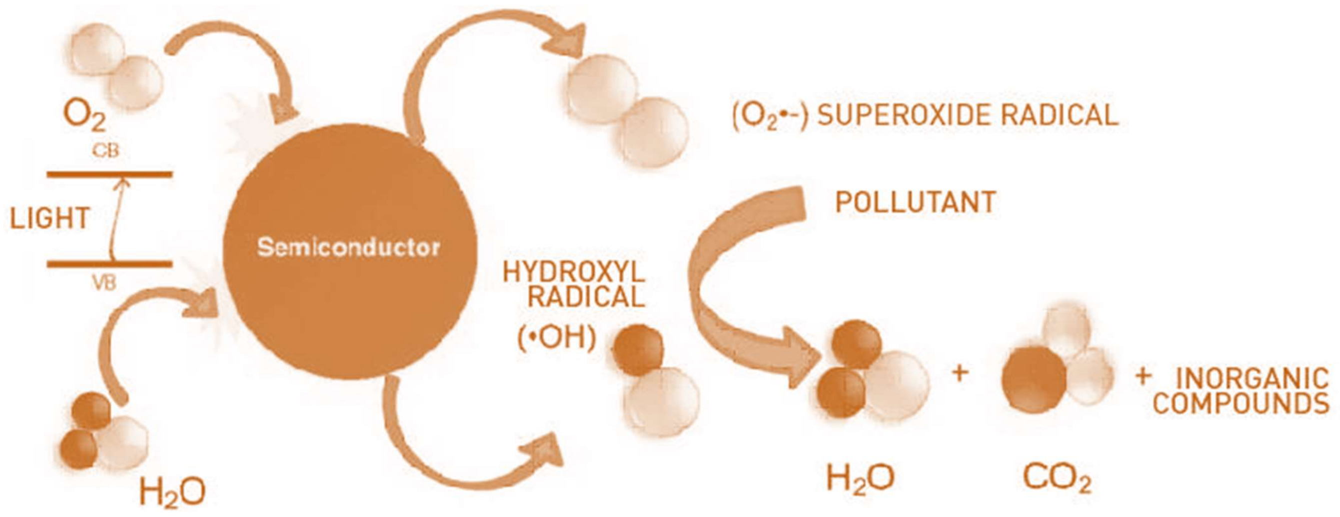


SCIENTIFIC BASIS

THE SCIENTIFIC BASIS OF h2o.TITANIUM

The objective of h2o.TITANIUM is to generate hydroxyl radicals through Advanced Oxidative Photocatalysis, a physico-chemical process capable of producing profound changes in the chemical structure of the contaminants, leadin to their mineralisation.

The catalyst, the h2o.TITANIUM reactor itself, is a wide bandgap semiconductor that is directly excited by the absorption of radiant energy, the photons are generated by the UV lamps it contains, so that, in the interface between the excited catalyst (titanium dioxide) and the solution (water and organic compounds mainly), the degradation reactions of the pollutants occur until they are mineralised.



Mechanism of the heterogeneous photocatalysis (Omo y Fitzpatrick, 2013, p. 191)

Titanium dioxide absorbs radiation in the near UV spectrum (< 380 nm) producing electron-hole pairs.

In the presence of redox species, adsorbed on the semiconductor particle and illuminated, oxidation and reduction reactions occur simultaneously on the internal surfaces of the reactor; the photo-generated holes give rise to photo-oxidation reactions, which produce hydroxyl radicals OH•.

$TiO_2(h^+) + H_2O_{ad} \rightarrow TiO_2 + OH\bullet_{ad} + H^+$

$TiO_2(h^+) + OH^-_{ad} \rightarrow TiO_2 + OH\bullet_{ad}$

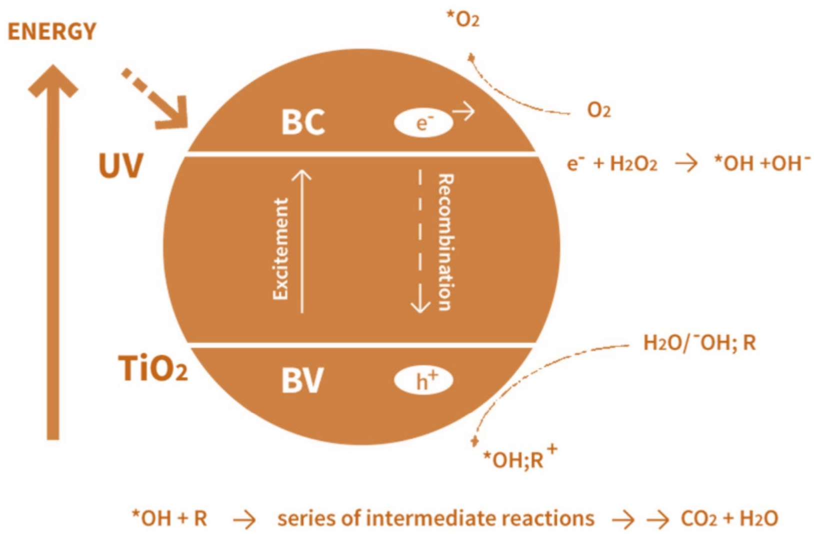
While the electrons of the conduction band give rise to photo-reduction reactions, which will be the trigger for the laterproduction of hydroxyl radicals OH•.

$TiO_2(e^-) + O_2 \rightarrow TiO_2 + O_2\bullet^-$

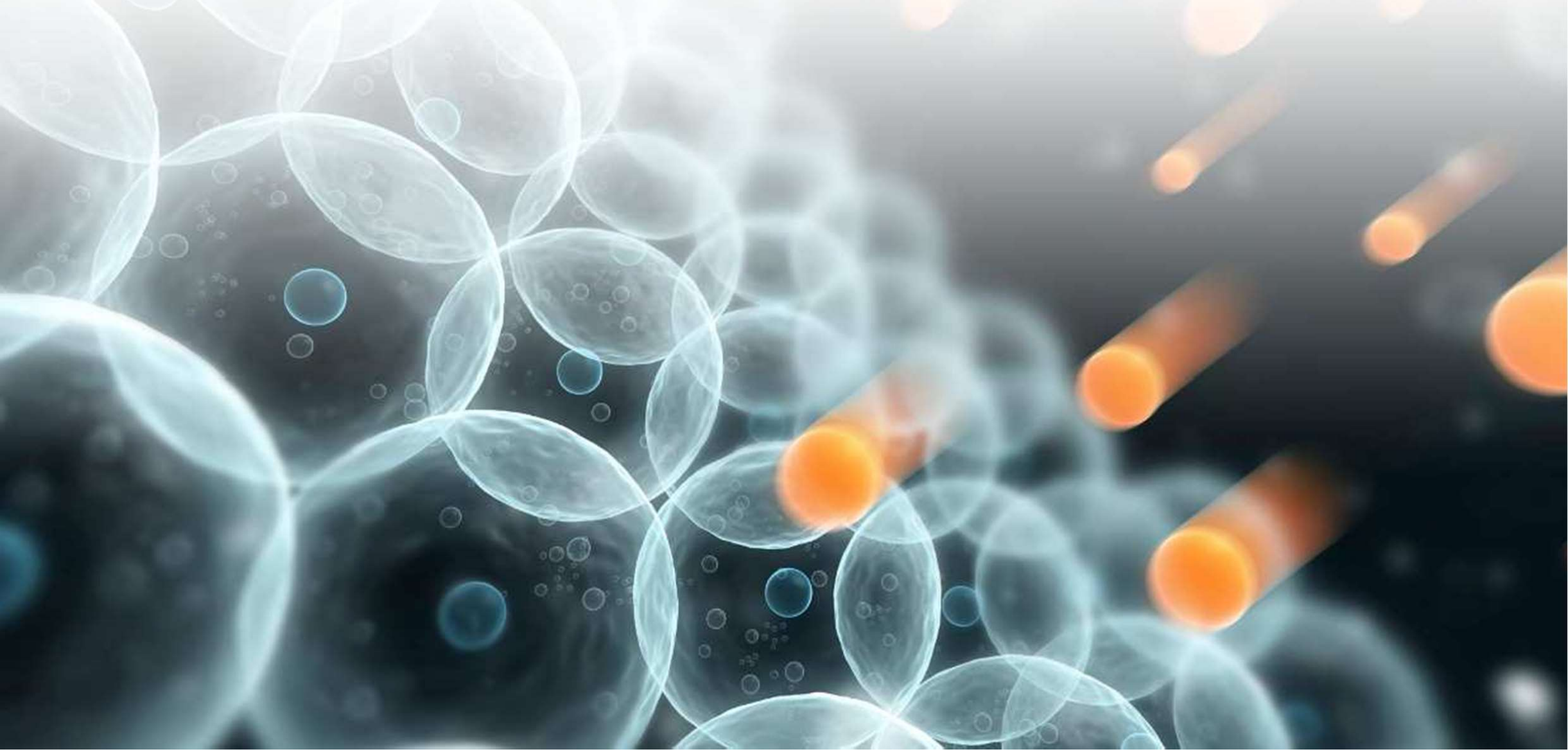
Molecular mechanism

The molecular orbitals of semiconductors have a band structure. The bands of interest for photocatalysis are the occupied valence band (VB) and the unoccupied conduction band (CB), separated from each other by the "energy spacing between bands" or "bandgap": (Ebg).

When the semiconductor is illuminated with photons (h) of higher energy than the bandgap (Ebg), an electron moves from the valence band into the conduction band, leaving a hole in the valence band.



The electron-hole pairs that are created have a half-life measured in nanoseconds, in that short time, they migrate to the surface and react with adsorbed species. The electron-hole pairs that do not manage to reach the surface and react with species there, recombine forming water and the energy dissipates.



The removal of organic matter from water by oxidizing agents follows a process that depends on the oxidizing agent's ability to withdraw electrons from the bonds constituting the molecules to be destroyed.

If they possess it, they can break each and every one of the bonds of the contaminating molecules, which, when oxidized, will have been transformed into CO2 and H2O. This is called mineralization. The redox potential of the agent defines its oxidative capacity. If it is not sufficient, no matter the quantity of oxidizing agent, as the redox potential does not increase with the concentration of oxidizing agents.

Since its redox potential is maximum, what the OH radical cannot oxidize (eliminate), no other oxidizing agent will be able to. The extremely short life of the OH radical means two things. One, that residual effect is not possible. Two, that everything occurs inside, and only inside, the reactor. And at a speed such that it is impossible to quantify.

Titanium dioxide is what is known as a wide-band semiconductor. When irradiated with the proper wavelength, it becomes activated (excitation of electrons – change of electronic band), triggering the generation of the OH radical. Please read the scientific article in the lower image for more detail.

However, there is **abundant scientific information** on this matter, dating back many years (Lawrence K., Norman C., Hung, 2005, for example).

Mechanism of the OH Radical Generation in Photocatalysis with TiO_2 of Different Crystalline Types

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Abstract