Development of photocatalyst based on Au/Pd@TiO2 nanoparticles by nano-QSPR and safe-by-design approaches

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Semiconductor heterogeneous photocatalysis is a versatile, low-cost, clean and environmentally benign treatment technology. TiO_2, especially in nanoparticle (NP) form, has been shown to promote the decomposition of a variety of organic and inorganic compounds. This implies its potential applications in sterilization, sanitation as well as air and water purification systems[1]. A drawback of titanium dioxide is that it can only be excited by ultraviolet light – thus extending its absorption wavelength range to the visible spectrum (VIS) through structure modifications is necessary.

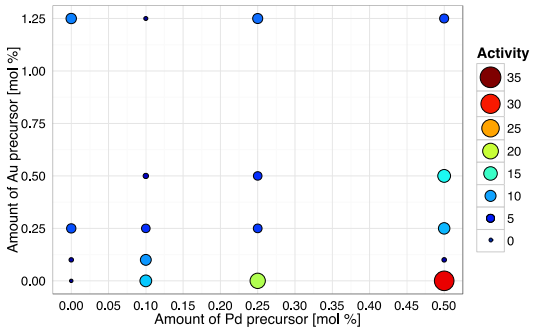

Fig.1 The photoactivity of mono and bimetallic nanoparticles at TiO_2 in phenol degradation after 1h irradiation under visible light (λ>420 nm).

Computational methods such as nanoscale *Quantitative Structure–Property Relationship* modeling for nanoparticles (nano-QSPR) might be a solution, combining the design of novel nanomaterials with potential environmental and human risk assessment[2, 3]. In our study of phenol degradation under VIS light (Fig.1), we have developed a nano-QSPR model for 16 Au/Pd@TiO_2 NPs, offering a meaningful mechanistic interpretation of their photocatalytic activity. The model, built using a combined GA-MLR (Genetic Algorithm - Multiple Linear Regression) technique, utilizes two molecular (empirical) descriptors and fulfills the required OECD recommendations (R^2=0.85, Q^2_{EXT}=0.81, Q^2_{CV}=0.74, CCC=0.89).

References

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