

Dual adsorbent-photocatalytic Keratin-TiO₂ nanocomposite for trimethoprim removal from wastewater.

María Emilia Villanueva^{a,b,c}, Mayra Puca^a, Jonás Perez Bravo^b, Jonathan Bafico^a, Viviana Campo Dall'Orto^{a,b} and Guillermo Copello^{a,b,*}

^a*Universidad de Buenos Aires (UBA), Facultad de Farmacia y Bioquímica, Departamento de Química Analítica y Fisicoquímica, (UBA), Junín 956, C1113AAD, Buenos Aires, Argentina;*

^b*Instituto de Química y Metabolismo del Fármaco, Facultad de Farmacia y Bioquímica, Universidad de Buenos Aires (IQUIMEFA-UBA-CONICET);*

^c*Universidad Nacional de Luján (UNLu) Departamento de Ciencias Básicas, Ruta 5 y 7 Luján, Buenos Aires, Argentina.*

*Corresponding Author: E-mail: gcopello@ffyb.uba.ar (G.J. Copello)

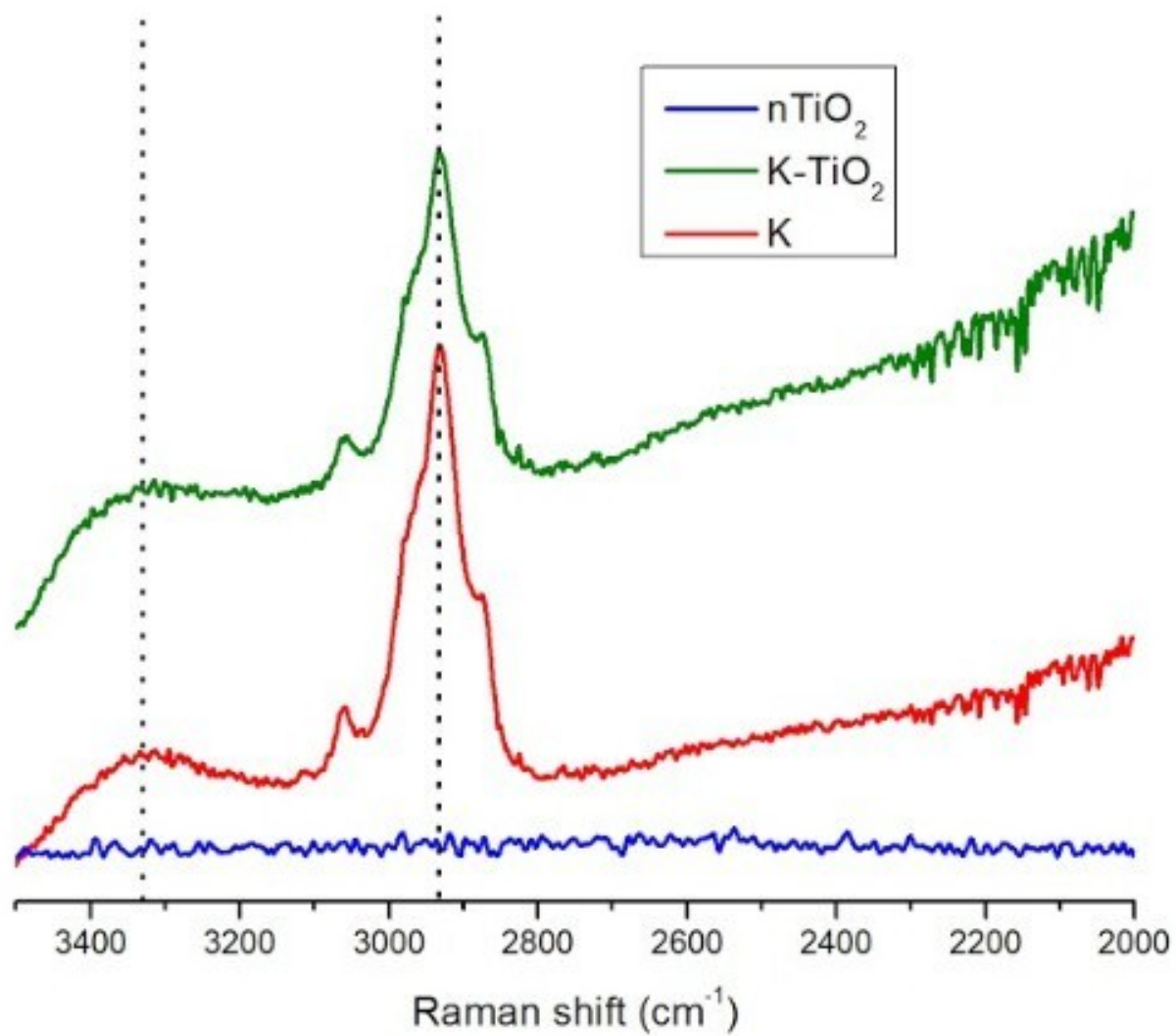


Figure S1. FT-Raman spectra of nTiO_2 , K and K-TiO_2 10%.

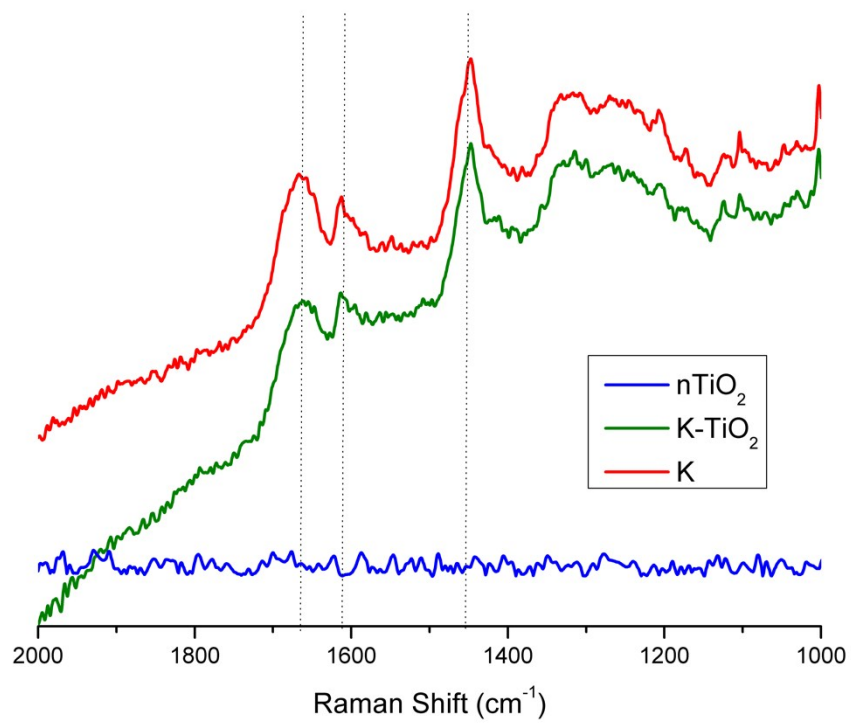


Figure S2. FT-Raman spectra of nTiO₂, K and K-TiO₂ 10%.

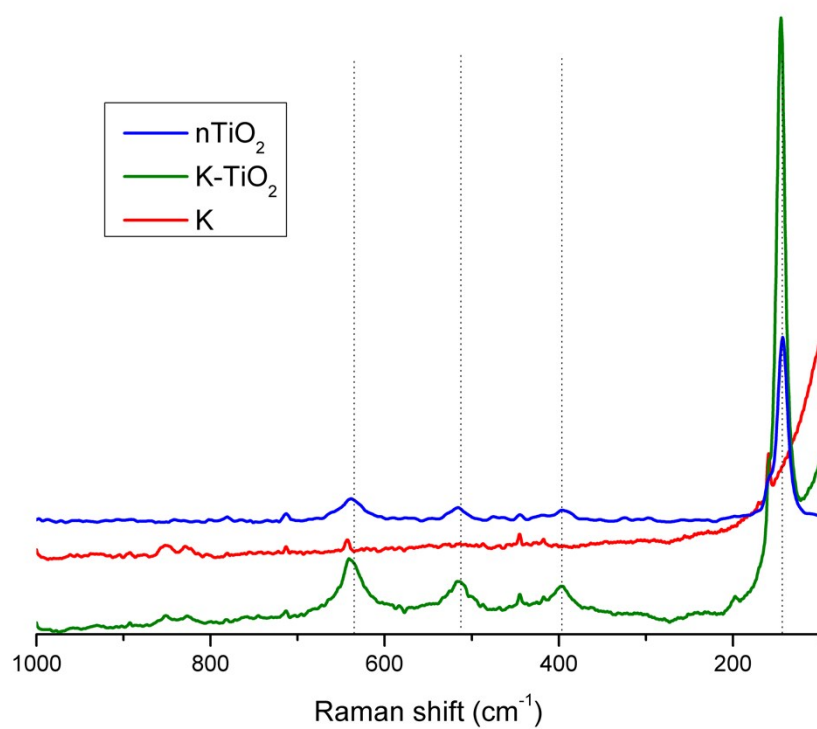


Figure S3. FT-Raman spectra of nTiO_2 , K and K-TiO_2 10%.

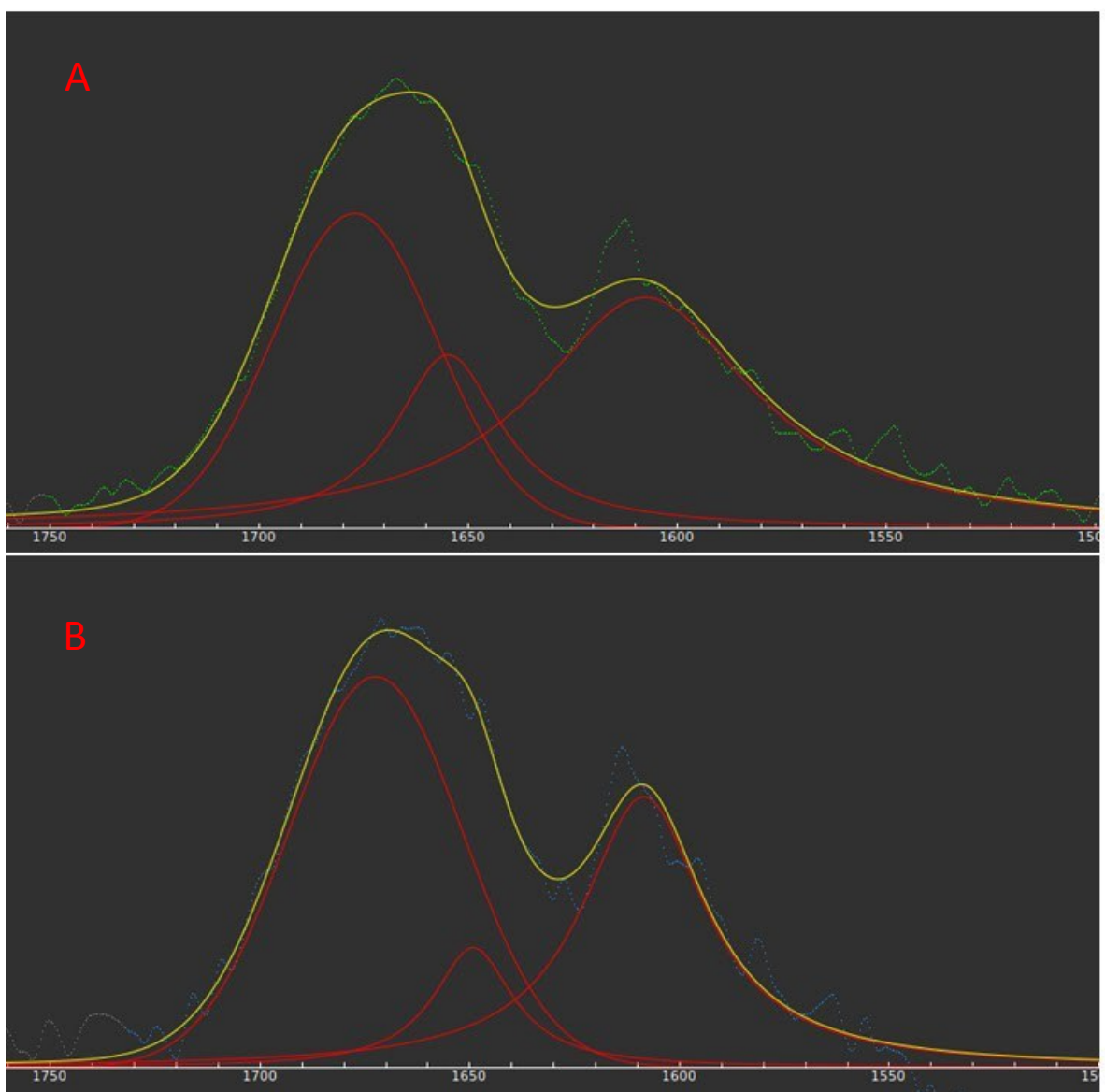


Figure S4. Deconvolution of amide I band in A) K and B) K-TiO₂ 10 %

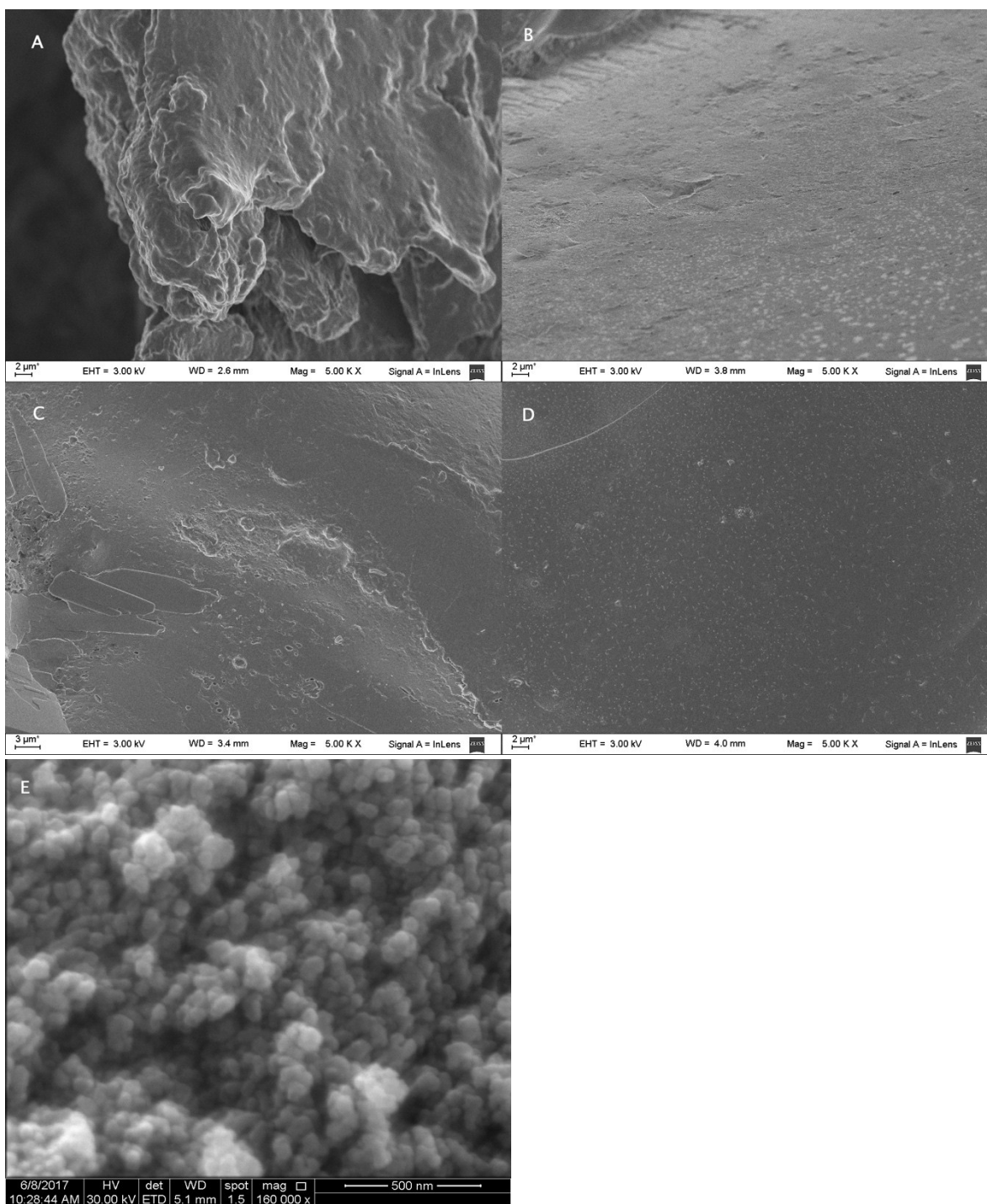


Figure S5. SEM Images of A: K, B: K-TiO₂ 1%, C:K-TiO₂ 5% and D: K-TiO₂ 10%, E:nTiO₂

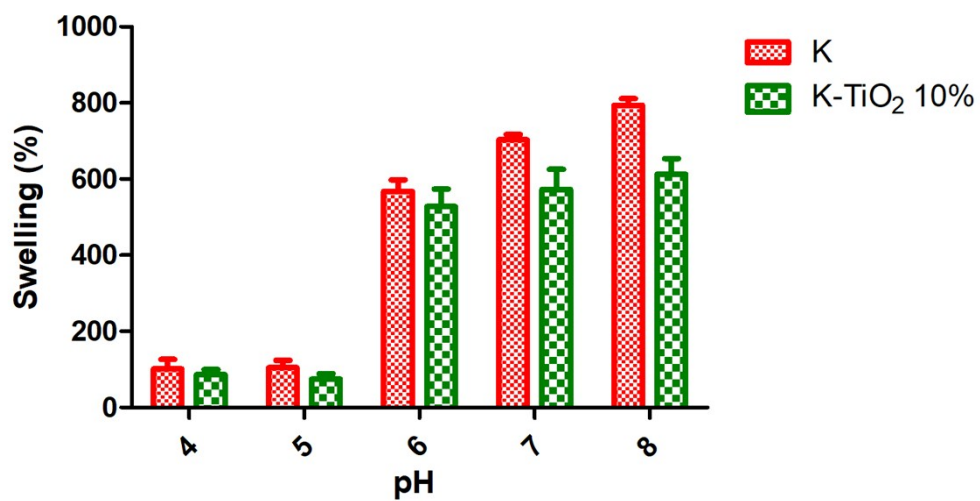


Figure S6. Swelling (%) of K and K-TiO₂ 10% at different pH values.

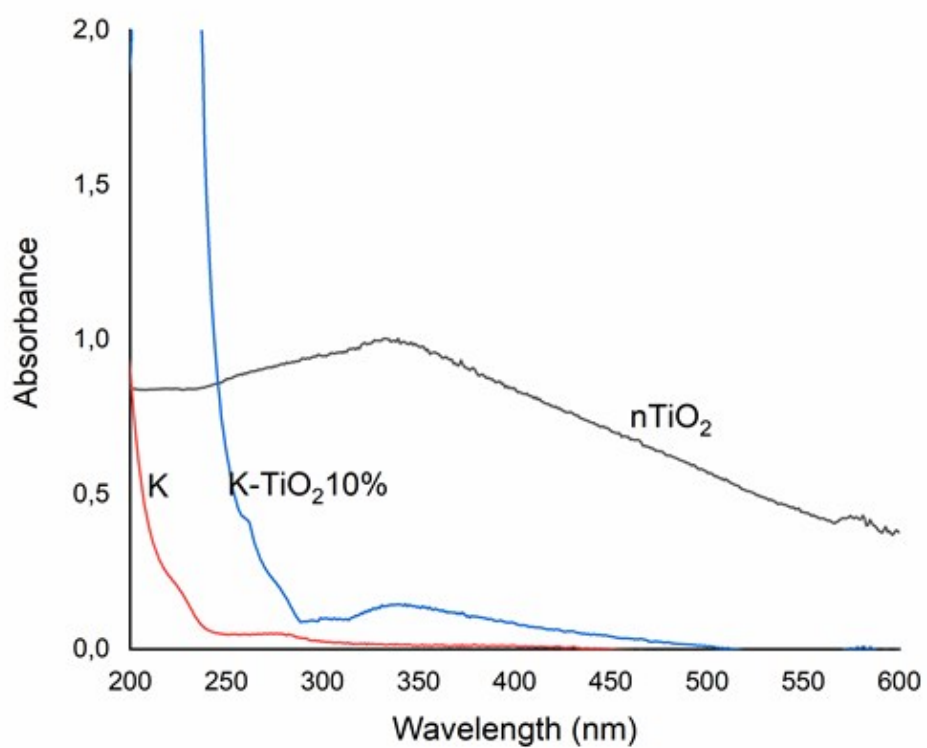


Figure S7. UV-Vis spectra of nTiO₂, K and K-TiO₂ 10%

Fig

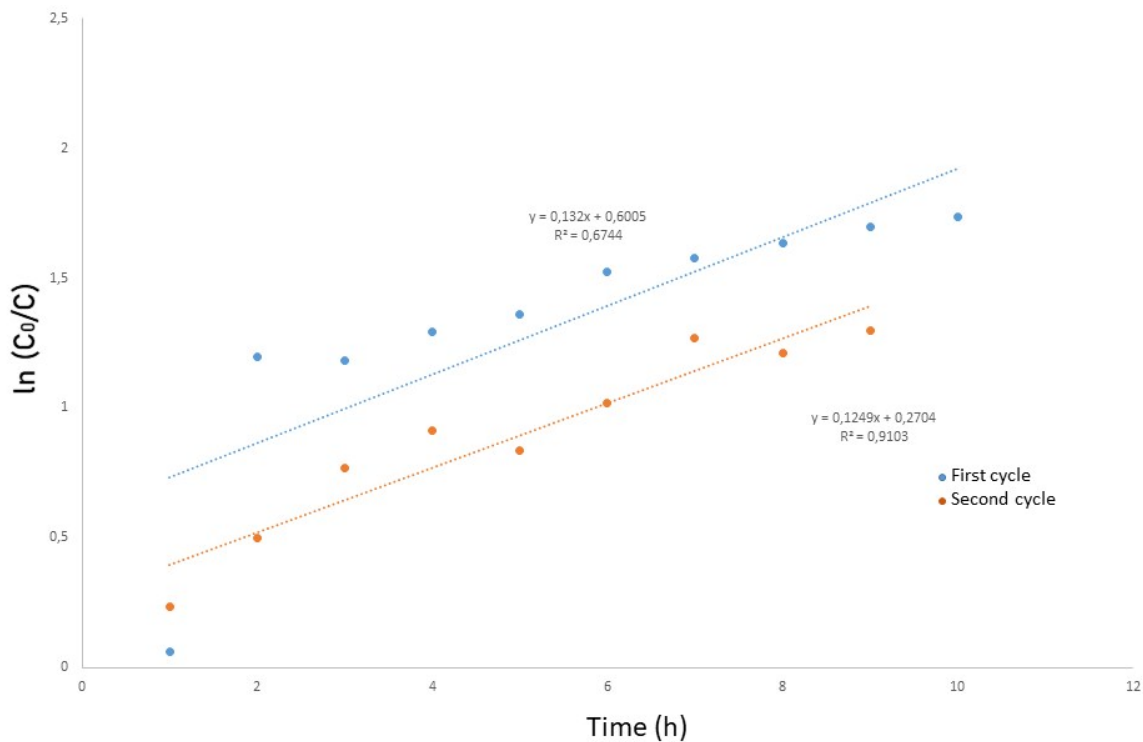


Figure S8. Degradation kinetics of Trimethoprim with K-TiO₂ 10% the first and the second cycle; showing apparent rate constants (slope = k_{app}) and regression coefficients (R^2).

Kinetic model

The Langmuir-Hinshelwood (L-H) kinetics model is often used to describe the photocatalytic degradation of pollutants (Eq.1)^{1,2}

$$r = \frac{dC}{dt} = \frac{kKC}{1+KC} \quad (1)$$

where r is the degradation rate of the reactant, C the trimethoprim concentration, t the illumination time, k the reaction rate constant, and K is the adsorption coefficient of the reactant.

If the initial Trimethoprim concentration (C_0) is a milimolar solution the equation can be simplified to an apparent first-order equation (Eq 2):

$$\ln \frac{c_0}{c} = kKt = k_{app} t \quad (2)$$

The graphic of $\ln C_0/C$ versus time represents a linear function which slope is the apparent first - order rate constant k_{app} .

The L-H model was designed to explain the dependence of the reaction rate with the initial pollutant concentration. The L-H expressions are useful to describe the photocatalysis in any of the following four situations: (a) the reaction occurs when both the radicals and the pollutant are adsorbed to the surface, (b) the reaction takes place between a radical attached to the surface and the pollutant molecule is in the solution, (c) the reaction happen when the pollutant molecule is linked to the catalyst and the radical is in the solution and (d) the reaction occurs when both species are in solution. In all the situations, the rate equation is similar to that derived from the L–H model, which has been useful to describe the process, although it is not possible to find out whether the process occurs on the surface, in the solution or at the interface.

1 M. E. Villanueva, G. J. Copello and V. C. Dall’Orto, *New J. Chem.*, 2018, **42**, 15405–15412.

2 N. Guettaï and H. Ait Amar, *Desalination Environ.*, 2005, **185**, 439–448.