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The adsorption and photo-degradation of oxalic acid at the TiO_2 surface. CECILIA MENDIVE, Universitaet Hannover, Germany, MIGUEL BLESA, CNEA, Argentina, DETLEF BAHNEMANN, Universitaet Hannover, Germany — Oxalic acid is the simplest model compound to study the heterogeneous photocatalytic oxidation of pollutants on TiO_2 containing more than one carboxylate group. We have carried out a study of a system of an oxalic acid solution in contact with a thin film of TiO_2 particles employing ATR - FTIR in combination with quantum chemical calculations. Thus, possible adsorption structures have been identified and molecular dynamic simulations have been used to compare their predictions with the experimental data. It was found that the adsorption of oxalic acid on TiO_2 in the dark can be explained in terms of two surface complexation modes for the anatase phase and only one surface complexation mode for the rutile phase. We have found that under illumination one of the complexes on the anatase phase preferably undergoes photo-degradation. At the same time water molecules are desorbed from the TiO_2 surface by a thermal mechanism induced by the absorption of photons. Both processes favor the adsorption of more molecules of oxalic acid at the TiO_2 surface which is thus enriched in the second complexation mode. A similar mechanism was found to occur on the rutile phase. The only complexation mode appears not to be photo-sensitive but the TiO_2 surface is enriched in oxalic acid under illumination due to the replacement of photo-desorbed water molecules.

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