Title

Removal and photocatalytic degradation of methylene blue on ZrO2 thin films modified with Anderson-Polioxometalates (Cr3+, Co3+, Cu2+): An experimental and theoretical study

Abstract

In this work, several ZrO2 thin films modified with Anderson-type polyoxomolybdates (POMs) with general formula (NH4)6-n[XMo6O24H6]-6+n where X = Co3+, Cr3+ and, Cu2+ were prepared. Thin films were characterized through SEM and EDX assay, UV–Vis diffuse reflectance and Fourier Transform Infrared (FTIR) assay. The optical bandgap of ZrO2 thin films was determined to be 3.25 eV, while the modified thin films showed a red shift in the optical activity compared with bare ZrO2 thin films. Methylene Blue (MB) adsorption studies showed that Freundlich isotherm describes properly the experimental data for modified-ZrO2 thin films. Besides, the kinetic results showed the MB adsorption of modified-ZrO2 thin films was superior to bare ZrO2 thin film. The adsorption rate values (K2) of the pseudo-second order model follow these trend ZrO2/CrPOM > ZrO2/CoPOM > ZrO2/CuPOM > ZrO2. The photocatalytic activity of the thin films for MB decomposition under UV and Visible irradiation was studied. Among all the catalysts, the ZrO2 thin films showed the lowest photocatalytic degradation rate kap value (kap = 1.5 × 10−3 min−1), while the best result was obtained for ZrO2/CrPOM thin films (kap = 5.7 × 10−3 min−1) under UV irradiation. Besides, this was the only catalyst efficiently active in MB degradation under visible irradiation, these materials reach 10.4 % after 100 min under visible irradiation. Finally, chemical calculations supported the observed results, by means of TDDFT, EDA analysis, Fukui function and periodic DFT calculations. © 2024 Elsevier B.V.

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