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BOOK OF ABSTRACTS

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Electrochemical Degradation of Phenols on PbO_2/Graphene Nanoribbons Electrodes – a Combined Experimental and DFT Approach

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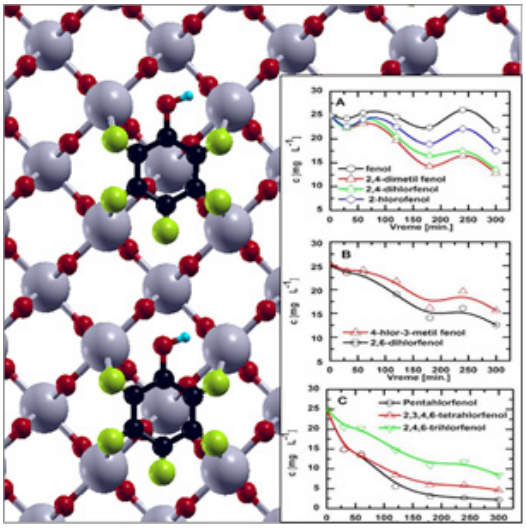

Electrochemical degradation of organic pollutants represents a promising technology for the depollution of waste water in the future. The concept comprises that the harmful pollutants are fully degraded into carbon dioxide and water using only electrical current, without any extra chemicals involved and with zero remnant waste [1]. The precise design of electrode materials, which should be highly efficient in generation of oxidizing OH radical and resistant to corrosion in applied electrochemical conditions, as well as careful control of experimental conditions, are of primary interest to achieve this goal [2,3]. Also, sophisticated and complex degradation pathways require knowledge on the fundamental principles beyond the oxidation process, in order to assure favourable outcome of the process and avoid formation of unwanted byproduct species.

In this contribution, a nanocomposite anode based on PbO_2 and graphene nanoribbons (PbO_2/GNR) was used for electrochemical oxidation of a mixture of phenol and chlorinated phenols. 0.1 M Na_2SO_4 (at pH = 3) was used as a supproting electrolyte. Tracking of phenols concentration revealed a degradation by up to 91 percents within 300 minutes at potential 2.3 V. The best degradation efficiency (91.4 %) was obtained for pentachlorphenol – a compound with the highest number of chlorine atoms, while the removal of phenol has achieved about 12%. Chromatographical tracking of degraded compounds has shown a rather complex oscillatory kinetics of phenol and trichlorphenols degradation, while pentachlorphenol concentration has been decreasing constantly within electrolysis.

The findings were complemented with periodic density functional theory (DFT) calculations of phenol and pentachlorphenol adsorption properties on the electrode surface models – PbO_2 crystal and graphene sheet. According to the obtained results, no adsorption of any of the investigated compounds on PbO_2 surface was observed. However, adsorption of phenol on graphene was thermodynamically favorable, while pentachlorphenol did not exhibit affinity for adsorption on graphene. Obtained theoretical and experimental results corroborate indirect mechanism of electrooxidation, where electrogenerated OH radicals on the electrode boundary initiate the oxidation of phenol and chlorophenols, resulting in subsequent generation of chlorine radicals and hypochlorite anions - which further continue to oxidize the species in the solution. Observed affinity of phenol to be adsorbed on graphene, which is the component of the anode, is among the possible causes of its low removal efficiency compared to the chlorinated phenols.

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