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Catalytic activity of nanostructured carbon electrodes for electrosynthesis of H_2O_2 through water oxidation: Predictions from first principles

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Abstract: H_2O_2 is a widely used reactant in industry, and a perfect agent for waste water treatment and drinking water preparation. H_2O_2 production via the electrocatalytic two-electron water oxidation reaction (2e WOR) is preferable to the presently used anthraquinone industrial process. The main challenge is to achieve selectivity of 2e WOR versus the competing 4e WOR which results in the O_2 gas evolution. At the moment the reaction conditions for selective 2e WOR remain mainly unknown, even though, different metal oxide electrodes, i.e. ZnO, MnO_2, SnO_2, WO_3, TiO_2, IrO_2, $BiVO_4$, were studied both theoretically and experimentally. Even though, some materials exhibited catalytic activity, further search for a better catalyst is still actual, due to limited chemical stability in aggressive H_2O_2 media and/or lack of selectivity.

In our study the carbon-type nanostructured electrodes for 2e WOR were studied from first principles by means of density functional theory. Calculated free energy of 2e WOR intermediates' adsorption and calculated overpotential required for successful 2e WOR are used as descriptors for comparing carbon-type thin films, their possible morphologies and reconstructions. The results are presented in both free energy diagrams and the volcano plot diagrams for graphene, bilayer graphene, diamond, and B-doped diamond. Our study provides deeper understanding of the catalytic properties of the carbon allotropes and influence of dopants on 2e WOR.

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