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DFT STUDY OF THE ENTIRE REACTION CYCLE OF H_2O_2 DECOMPOSITION AND O_2 GENERATION CATALYZED BY FENTON REAGENT

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Abstract. The reaction cycle of H_2O_2 decomposition and O_2 generation catalyzed by Fenton reagent was studied using density functional theory calculations. A four-stage mechanism for the oxygen production and the Fe^{2+} regeneration in the Fenton reaction is proposed based on the obtained results. The transition state for each step of the entire reaction cycle was localized and verified by intrinsic reaction coordinate analysis. It is shown that the O-O bond cleavage of coordinated H_2O_2 at the first step of reaction does not lead to a free $HO^{\bullet}$ radical. Instead, a highly reactive intermediate $[Fe^{IV}(H_2O)_4(OH)_2]^{2+}$ with two $HO^{\bullet}$ radicals "trapped" in the complex is formed with the energy barrier of 15 kcal/mol. The result of the next two reaction steps is the formation of the two $HO_2^{\bullet}$ radicals which can react on the triplet energy surface in order to produce O_2 in the triplet ground state and a H_2O_2 molecule.

Keywords: Fenton reaction, H_2O_2 decomposition, DFT calculation.

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