**THEORETICAL INVESTIGATION OF OXYGEN REACTION WITH PALLADIUM PORPHYRIN**

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The main objective of the study was to investigate the palladium porphyrin reaction with oxygen with the use of quantum chemistry methods.

Many porphyrin complexes have been synthesized with transition metals. They are important in organic synthesis, catalysis, as a compounds in photodynamic therapy and many others [1]. In this work, palladium porphyrin was considered, which has a particularly interesting property: the phosphorescence is quenched in the presence of oxygen and makes it potential oxygen sensing agents [2]. Through the reaction of the porphyrin ring with oxygen, this compound is able to produce oxygen in the singlet state [3].

The calculations, were performed by DFT and TD-DFT methods using PBE0 functional. The def2-TZVPP basis sets was used and the presence of water as a solvent is taken into account using PCM model solvent.

In calculations, all possible combinations of oxygen attachment to the porphyrin ring were considered and expected structures were fully optimized. The obtained structures can divided into two groups. First of them (I) is characterized by slightly elongated O-O bond and oxygen atoms are attached to neighboring carbon atoms of porphyrin ring. In second group (II) the O-O bond undergoes breaking. Products with O-O bond broken are the most stable. Direct connection of oxygen molecule to palladium is energetically unfavorable. The calculation predict that in first step of reaction the structure of type I should be produced, which subsequently can converted to structure of type II. On alternate reaction path, the Pd(II)por-O2 complex can be decay with formation of oxygen molecule in singlet electronic state.

**References**

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