# The reaction mechanisms between atomic oxygen and water using high-level quantum mechanical calculations

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Electric gas discharge plasmas generated in oxygen containing gas mixtures, such as air or oxygen admixed with noble gases, produce atomic oxygen in either the ground triplet state, $O(^3P)$, or the excited singlet state, $O(^1D)$ [1-3]. In contact with humidity or with aqueous solutions, oxygen atoms may undergo reactions with water molecules, or may dissolve in solutions and undergo reactions in the liquid phase [4-8]. These reactions are crucial for plasma processing of liquids and biological molecules for diverse applications in health and environmental remediation. In addition, these reactions are broadly involved in environmental and atmospheric chemistry.

Despite their significance, the detailed reaction mechanisms involving oxygen atoms in the presence of water are not completely understood. Yusupov *et al.* [9] investigated the interaction of atomic oxygen with liquid water using ReaxFF molecular dynamics simulations wherein abstraction of a hydrogen atom from a water molecule was predicted with subsequent formation of two OH radicals. Verlackt *et al.* [10] predicted the formation of oxywater as a result of interaction of singlet states oxygen atoms with water using density functional tight binding (DFTB)-based molecular dynamics simulations which was stable for 10 ps of simulation time. Xu *et al.* [11] predicted the formation of oxywater as the intermediate product in the interaction between singlet state oxygen atom and water using density functional theory (DFT)-based molecular dynamics simulations. This was followed by the generation of hydrogen peroxide as the final product.

The past controversial outcomes motivated us to explore the reaction mechanisms between oxygen atoms and water molecules using high-level quantum mechanical calculations. The results will be presented in this talk.

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