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Oxidation and Advanced Oxidation processes in water and wastewater treatment

Keynote Speaker
Peter Tentscher, *Department of Chemistry and Bioscience Aalborg University, Denmark*

"Oxidative micropollutant abatement: Options and limitations of quantum chemical computations"

Oxidation processes are important for the abatement of micropollutants and lead to corresponding transformation products. Wastewater and drinking water treatment may employ oxidation for targeted removal of micropollutants, whereas in surface waters, photooxidation contributes significantly to the natural attenuation of these compounds. Owing to the high number of micropollutants, it is impossible to experimentally assess the abatement of every compound in every setting. It is thus necessary to understand the reaction mechanisms of these reactions, and to develop predictive models for the reaction kinetics- knowledge that is transferable from one compound to another. Quantum chemical calculations can help to evaluate proposed reaction mechanisms by estimating their thermodynamic and kinetic feasibility. Thermodynamic feasibility can be evaluated by Gibbs free energy calculations of the involved reactants, intermediates, and products. A proposed reaction mechanism should ideally involve species that are connected on a potential energy surface formed by atomic coordinates, allowing also the estimation of the free energy of activation of a reaction. Also, quantum chemical descriptors such as orbital energies can be used to construct quantitative structure-property relationships (QSPRs) to predict second order rate constants for oxidation reactions. In this talk, an overview of the corresponding quantum chemical methodologies will be given, and some representative examples from ozonation reactions will be presented.