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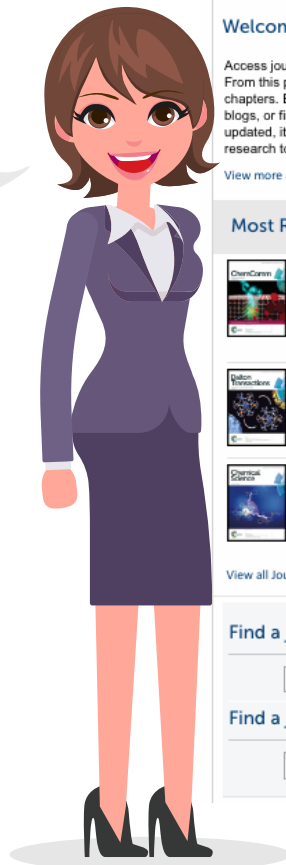


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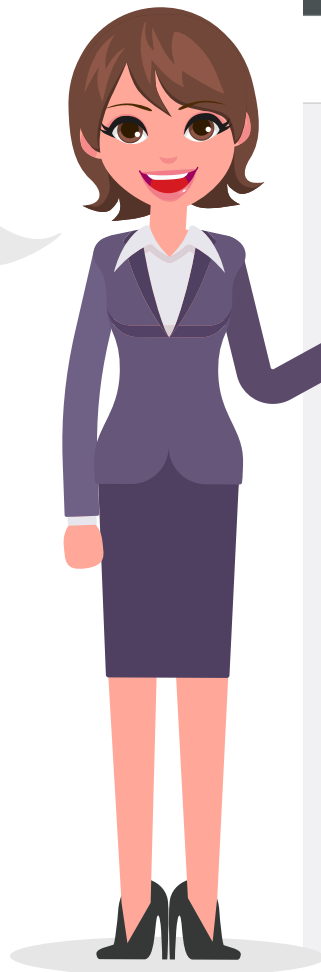
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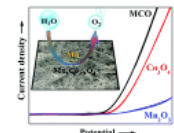
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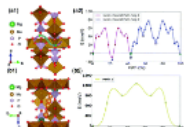


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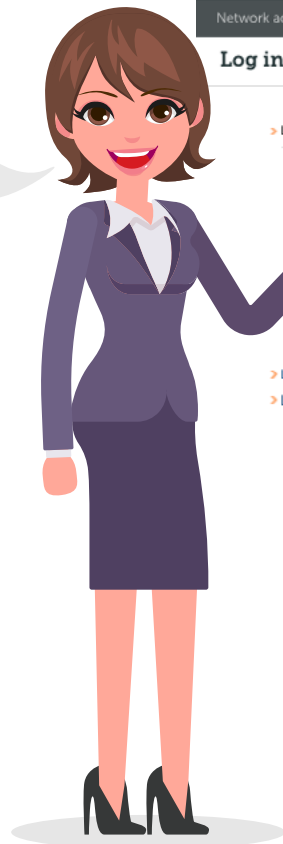
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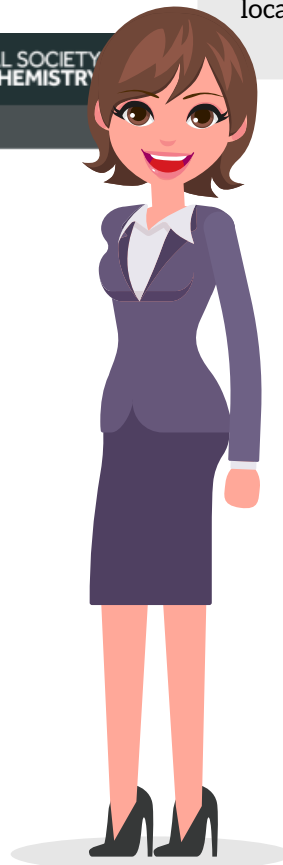
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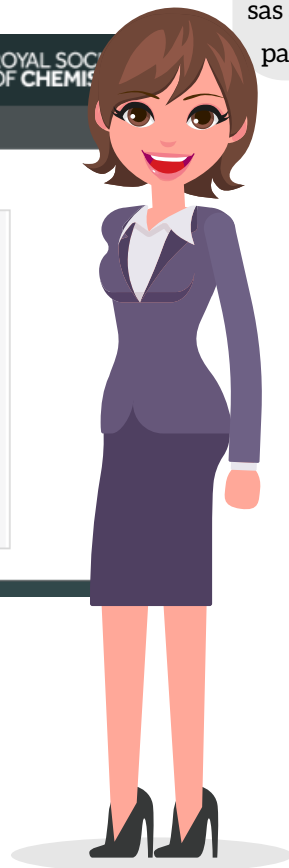
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[Yunho Lee](#)^a and [Urs von Gunten](#)^{a,bcd}

 [Author affiliations](#)

Abstract

Ozonation of municipal wastewater effluent has been considered in recent years as an enhanced wastewater treatment technology to abate trace organic contaminants (micropollutants). The efficiency of ozonation for micropollutant abatement depends on (1) the reactivity of ozone and OH radical ($\cdot\text{OH}$) with the target micropollutant, (2) the dosage of ozone and the stability of ozone and $\cdot\text{OH}$ in a given water matrix, (3) the removal of undesirable effects (e.g., biological activities) of a micropollutant after structural transformation, and (4) the biodegradability of transformation products in biological post-treatment. In this article, recent advances in predicting organic micropollutant abatement during ozonation of municipal wastewater effluents are reviewed with a focus on (i) principle-based approaches for describing and modeling the reaction kinetics of ozone and $\cdot\text{OH}$, (ii) transformation products and pathways, (iii) changes of biological activities, and (iv) biodegradation of transformation products in biological post-treatment. Using the chemical kinetics based on ozone and $\cdot\text{OH}$ rate constants (i.e., compound-specific information) and exposures (i.e., water matrix-specific information), a generalized prediction of the abatement efficiency of various micropollutants in varying water quality appears to be possible. QSAR-type correlations based on Hammett coefficients or quantum chemical energy calculations or (semi)empirical models have been developed for predicting the ozone and $\cdot\text{OH}$ rate constants and exposures, respectively. Models based on the ozone and $\cdot\text{OH}$ reaction rules can be used to predict the transformation products of micropollutants by ozone and $\cdot\text{OH}$. Reaction rule-based models in combination with the chemical kinetics information will enable the prediction of transformation product evolution during ozonation. The biological activities of transformation products have been assessed by an effect-driven approach using *in vitro* bioassays. Biological activities with specific modes of action (e.g., receptor-

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Advances in predicting organic contaminant abatement during ozonation of municipal wastewater effluent: reaction kinetics, transformation products, and changes of biological effects

Yunho Lee^{*a} and Urs von Gunten^{*bcd}

Ozonation of municipal wastewater effluent has been considered in recent years as an enhanced wastewater treatment technology to abate trace organic contaminants (micropollutants). The efficiency of ozonation for micropollutant abatement depends on (1) the reactivity of ozone and OH radical ([•]OH) with the target micropollutant, (2) the dosage of ozone and the stability of ozone and [•]OH in a given water matrix, (3) the removal of undesirable effects (e.g., biological activities) of a micropollutant after structural transformation, and (4) the biodegradability of transformation products in biological post-treatment. In this article, recent advances in predicting organic micropollutant abatement during ozonation of municipal wastewater effluents are reviewed with a focus on (i) principle-based approaches for describing and modeling the reaction kinetics of ozone and [•]OH, (ii) transformation products and pathways, (iii) changes of biological activities, and (iv) biodegradation of transformation products in biological post-treatment. Using the chemical kinetics based on ozone and [•]OH rate constants (*i.e.*, compound-specific information) and exposures (*i.e.*, water matrix-specific information), a generalized prediction of the abatement efficiency of various micropollutants in varying water quality appears to be possible. QSAR-type correlations based on Hammett coefficients or quantum chemical energy calculations or (semi)empirical models have been developed for predicting the ozone and [•]OH rate constants and exposures, respectively. Models based on the ozone and [•]OH reaction rules can be used to predict the transformation products of micropollutants by ozone and [•]OH. Reaction rule-based models in combination with the chemical kinetics information will enable

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