

## **Development of a Toolbox for Property and Fate Prediction of New and Emerging Contaminants Based on Thermodynamic Modeling**

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**Abstract.** Numerous anthropogenic chemicals have been and are being released into the environment. For many new and emerging contaminants, properties that govern their fate in both natural environments and engineered remediation systems are unknown. The classical approach of conducting treatability studies, however, is highly time- and money-consuming. This creates a need for a predictive tool that allows scientists, consultants, and regulators to rapidly identify a suitable and cost-effective way of dealing with these substances.

The objective of this project is to develop a model that can be used to screen new and emerging contaminants such that treatment options and potential problem intermediates can be identified. As a first approach, quantum mechanical modeling will be used to derive thermochemical parameters relevant for predicting chemical reactivity such as free energies of formation and reaction, bond dissociation energies, HOMO/LUMO energies etc. Modeled parameters and relationships will subsequently be confirmed experimentally via electrochemical and/or spectroscopic techniques. Ultimately, the model will be validated on a bench and field scale.