AI/ML-Assisted Advancement of Degradation Science of Per- and Polyfluoroalkyl Substances (PFAS) on 2-Dimensional Nanoconfining Substrates

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Project Summary: Hyperconjugation causes helicity in longer chain per- and polyfluoroalkyl substances (PFAS) which can be alleviated by dispersive interactions with 2D substrates such as Al2O3. Advanced oxidative (persulfate-driven) and reductive (hydrated electron-driven) processes can accelerate the degradation of such non-helical PFAS due to regained accessibility to □□□□□ internal C-C bonds, and nanoconfinement. In this regard, the vast degradation reaction space necessitates the use of ML methods for availing optimal reaction conditions. Sequential steps of 3D featurization using voxelization, 2-point correlation, principal component analysis and Gaussian process regression can minimize the uncertainty and provide sensitivity of PC scores of multi-component system leading to more effective PFAS degradations. Such research can enhance the legacy response of DoD to this environmental and human health crisis, and further lead to the application of the science to other hyperconjugation-possessing systems.
