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Goethite-Bound Copper Controls the Fate of Antibiotics in Aquatic Environments

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The coadsorption of Cu(II) and quinolones to goethite (GT) surface strongly affect their fate in the natural environment via cooperative binding, little is still known about the interaction information at molecular level, the different adsorption behavior of Cu(II) facing different quinolones and vice versa, and the final fate of quinolones adsorbed on GT. In this study, we addressed these issues by describing the adsorption or oxidation behavior of Cu(II) and zwitterionic ciprofloxacin (CIP) or non-zwitterionic fluoroquinoloic acid (FOQA) onto GT under different environmental conditions (pH, ionic strength, concentration etc.). We found that the CIP uptake was greatest at circumneutral pH and in saline conditions, where Cu(II), CIP, and mineral surface charges were the least repulsive. Vibrational spectroscopy and molecular simulations revealed that the enhanced uptake of CIP was caused by the coordination of metal-bonded Cu(II)−CIP surface complexes on goethite. The inner-sphere Cu(II)−CIP complex also facilitated CIP oxidation into a series of new products, which we identified by mass spectrometry. Finally, to predict Cu(II) and quinolone loadings prior to redox-driven reactions, we propose a multisite surface complexation model using Cu(II)−CIP ternary surface complexes, alongside an ion pair to account for the ionic strength dependence on loadings. The information developed in this work will help tracking the fate of CIP in contaminated aquatic environments.