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Decoding the Environmental Coating of TiO_2 Nanoparticles: Insights from Complementary Surface Analytical Techniques

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Understanding the fate and transport of natural colloids and engineered nanoparticles in aquatic systems requires detailed insight into their interactions with natural solutes forming environmental coatings on their surfaces. The properties of these coatings—such as hydrophobicity, surface charge, and thickness—govern particle behavior, including interactions with natural substrates, pollutant sorption, and colloidal stability. Characterizing these complex and potentially heterogeneous coatings therefore remains crucial to predict colloid behavior and ecological impacts in natural waters. A complete description necessitates complementary surface characterization techniques.

Here, we evaluate the potential and limitations of X-ray photoelectron spectroscopy (XPS), laser desorption/ionization Fourier-transform ion cyclotron resonance mass spectrometry (LDI-HRMS), time-of-flight secondary ion mass spectrometry (ToF-SIMS), infrared spectroscopy (IR), thermogravimetry coupled to mass spectrometry (TGA-MS), and atomic force microscopy (AFM) to characterize environmental coatings on five types of TiO_2 nanoparticles representative of those used in paints and sunscreens. Pristine particles and particles extracted from commercial products were exposed to contrasting surface waters in situ using the dialysis bag method to generate environmental coatings.

Combined analysis revealed that coating composition tends to cluster by particle type and sampling site, particularly in waters with distinct chemical features such as high dissolved organic matter (DOM) or Ca^{2+} concentrations. As expected, coatings displayed complex compositions. LDI-HRMS proved most sensitive to variations in molecular fingerprints and effectively clustered samples by DOM characteristics, while XPS and ToF-SIMS reflected differences related to the pristine surface coating. These discrepancies are discussed in light of each technique's measurement principles. Although IR and TGA-MS provided limited analytical depth, both confirmed carbonate presence and complemented XPS data. Notably, TGA-MS uniquely provided quantitative estimates of organic matter content. AFM showed promise for probing nanoscale hydrophobicity, though further methodological advancements are required.

Overall, the environmental coating composition is strongly influenced by the particle's original coating and aging history, except in peatland or calcareous waters where autochthonous matter dominates. This study presents, to our knowledge, the first comprehensive in situ characterization of environmental coatings, and recommends a combined approach using XPS, LDI-HRMS, TGA-MS, and IR, with careful interpretation of the resulting complex datasets.