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High-Throughput Quantification of Soil Organic Carbon and Mineral Carbon Capture with Fluorescence-Free Raman Spectroscopy and Machine Learning

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Data-driven precision agriculture, environmental stewardship, and terrestrial carbon capture require accurate means for the chemical analysis of soil systems at scale. Traditional measurement methods, such as combustion analysis for soil organic carbon (SOC), provide accurate results but are slow, resource-intensive, and unsuitable for field deployment. Raman spectroscopy combined with machine learning offers a rapid and field-deployable alternative to conventional measurements. However, Raman measurements of such samples are challenged by fluorescence, particle size variation, and heterogeneity. Here, we address these issues in a novel approach to the quantification of organic carbon in farm soils and mineral carbon capture in brucite ($Mg(OH)_2$) using Raman spectroscopy with machine learning. Central to this approach is a custom-built Shifted-Excitation Raman Difference Spectroscopy (SERDS) instrument that integrates specialized optical design, signal-processing algorithms, and machine-learning analysis.

We quantified SOC in 400 U.S. farm soil samples using machine-learning regression models trained on fluorescence-free SERDS spectra. These measurements reveal that Raman intensities vary nonlinearly with organic carbon content, particle size, and sample opacity, reducing the accuracy of conventional machine learning models. We introduce a novel SERDS pre-processing algorithm, in conjunction with a physics-informed machine learning framework that accounts for particle size variations and improves predictive accuracy.

We have extended this approach to quantify carbon capture in brucite ($Mg(OH)_2$), a mineral in ultramafic mine tailings that forms stable carbonates. SERDS, combined with nonlinear machine learning models, accurately measures the captured inorganic carbon. The SERDS method outperforms univariate band-based approaches, especially in the presence of variable fluorescence backgrounds. Further studies of the fundamental chemistry governing brucite carbon capture have employed *ab initio* molecular dynamics simulations. This theoretical investigation provides a unique view of the kinetics and thermodynamics of brucite-based carbon capture at the atomic level.

Overall, this work has combined spectroscopy, machine learning, and molecular modelling to address geochemical questions from atomic-level carbon capture chemistry to field-deployable soil and mineral analyses. By enabling rapid, high-throughput quantification of both organic and inorganic carbon, these methodologies will guide soil management practices, validate carbon capture in mining operations, and support the large-scale implementation of carbon sequestration strategies.