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# Raman Spectroscopy and Machine Learning for Carbon Capture Measurement in Magnesium Hydroxides

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As global greenhouse gas emissions rise, the mining industry offers potential for $CO_2$ capture in mine tailings and industrial byproducts. Brucite ($Mg(OH)_2$), found in ultramafic mine tailings and industrial byproducts such as cement and magnesia, captures $CO_2$ in a stable mineral-forming reaction. Current methods to quantify inorganic carbon (acidification, combustion) are time inefficient and destroy the sample, preventing further analysis. Efficient quantification of brucite carbon capture requires an automated, high-throughput technique. While existing Raman measurements of minerals can elucidate molecular structure and hydration level, they are challenged by non-uniform crystallinity, complex chemical composition, and background fluorescence. Here, we measure brucite carbon capture by correlating total inorganic carbon with fluorescence-free Shifted-Excitation Raman Differential Spectroscopy (SERDS) features using machine learning multivariate regression. Total inorganic carbon (TIC), determined by coulometric acidification, provides ground-truth values. Overall, non-linear models outperform linear models for carbonate prediction, particularly for single-output variable predictions. Univariate carbonate-band area-under-curve measurements correlate weakly with TIC. Particular nonlinearity appears for TIC > 6 wt% as a consequence of differences in crystallinity, hydration state, carbonate phase assemblage, and band overlap. Experiments testing the addition of simulated fluorescence further establish that nonlinear multi-parameter models outperform their linear counterparts. Mean absolute error increases by 0.76 and 0.46 for linear and nonlinear regression, respectively, with the addition of simulated fluorescence. Fluorescence-free Raman spectroscopy improves all machine learning models, especially complimenting stronger baseline performance of nonlinear models. By refining and scaling, we expect this approach to yield an effective, high-throughput means to validate new industrial carbon capture methods. In doing so, we aim to accelerate their widespread adoption.