

# Correlating Surface Area, Surface Chemistry and Light Absorption in Carbon Nitrides: Development of New Metrics for Comprehensive Characterization

Balasubramanian Viswanathan,<sup>1</sup> Harindranathan Nair,<sup>2</sup> HARIPRASAD NARAYANAN<sup>1,2</sup>

<sup>1</sup>National Centre for Catalysis Research, Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036

<sup>2</sup>School of Environmental Studies, Cochin University of Science and Technology

Email: hariprasadmamandur@gmail.com

This study introduces two novel parameters for advanced material characterization: the D Parameter to Surface Area (D.P/S.A) ratio and the Normalized Surface Concentration percentage (%NSC), developed and applied to graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) synthesized using various crucibles. The D.P/S.A ratio, derived from Second Derivative UV-Visible Diffuse Reflectance Spectroscopy (SD-UV-DRS) and surface area analysis, quantifies a material's light absorption efficiency relative to its surface area. It offers insights into the relationship between structural properties and optical characteristics, potentially predicting photon-utilization efficiency in various applications. The %NSC, calculated from X-ray Photoelectron Spectroscopy (XPS) and surface area analysis data, provides a normalized view of surface elemental composition and functional groups. By accounting for surface area variations, %NSC allows for more accurate comparisons of surface chemistry across samples with different morphologies or synthesis conditions. We demonstrate these parameters' application in analyzing g-C<sub>3</sub>N<sub>4</sub> synthesized using different precursors and methods. Our results show that D.P/S.A and %NSC effectively highlight subtle differences in material properties that conventional characterization methods might overlook. These metrics offer advantages over traditional techniques by providing a more nuanced understanding of material properties, bridging the gap between bulk and surface characteristics. This study aims to provide the scientific community with new tools for comprehensive material characterization, potentially leading to more informed material design and improved performance in diverse applications, including catalysis, photonics, and energy storage. The developed metrics have broad applicability in materials science, aiding in the optimization of synthesis processes and the prediction of material performance across various fields.

## References:

- [1] J. W. M. Osterrieth et al., How Reproducible are Surface Areas Calculated from the BET Equation?, *Adv. Mater.* 34, 2201502 (2022).
- [2] G. G. Terrones, Y. Chen, A. Datar, L.-C. Lin, H. J. Kulik, and Y. G. Chung, SESAMI APP: An Accessible Interface for Surface Area Calculation of Materials from Adsorption Isotherms, *J. Open Source Softw.* 8, 5429 (2023).
- [3] Dubrovkin, J., *Derivative Spectroscopy*; Cambridge Scholars Publishing: 2020.
- [4] Dubrovkin, J., *Data Compression in Spectroscopy*; Cambridge Scholars Publishing: 2022.
- [5] Dubrovkin, J., *Mathematical Processing of Spectral Data in Analytical Chemistry: A Guide to Error Analysis*; Cambridge Scholars Publishing: 2019.