Development and optimization of functional materials and their components are hindered by both the complex nature of the materials, a partial understanding of the relationship between performance, chemistry and morphological properties. XPS is one of the most widely utilized surface spectroscopic techniques for the analysis of materials because this technique allows discriminating between oxidation states of the elements. Surface morphology is one of the most important factors affecting the functional performance of components. Digital image processing of images can convert the 2-D and 3-D intensity distribution into 1-D image descriptors (values) that are utilized for quantitative morphology analysis. A vitally important for functional characterization must be an appropriate separation of the different components of surfaces, which is not only to extract roughness, waviness and form, but also should be extended to concern all multi-scalar topographical events over surface.

Predicting macroscopic properties of interest, such as activity and stability, from materials chemistry and structure is challenging yet feasible using a multianalytical approach combined with multivariate analysis. Correlation of structure, morphology, and performance through the application of multivariate analysis will be discussed for different families of inorganic and biological composite materials.