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Chemical Analysis of Commercial Functionalized Graphene along the Production Process

Graphene has found widespread commercial use, particularly in flexible electronics and coatings for substrates such as paper and textiles, in the form of suspensions and inks (Zhang et al., 2017). Functionalization of graphene allows fine-tuning of properties like electrical conductivity. Structural and chemical features of graphene materials are typically analyzed by Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). While Raman spectroscopy plays a critical role in identifying the presence of graphene and characterizing its structural defects (Pollard et al., 2017), XPS examines the chemistry of graphene. This study investigates three types of graphene materials — graphene (unfunctionalized, G-graphene), fluorine-functionalized graphene (F-graphene), and nitrogen-functionalized graphene (N-graphene) — across three physical forms: powders, suspensions, and embedded in inks. Functionalization was performed via plasma treatment of G-graphene with fluorine or ammonia gases. Suspensions were obtained by dispersing powders in distilled water, while inks were formulated using diacetone alcohol, carbon black, and graphene. Raman spectroscopy analysis confirmed the graphitic nature of all materials and revealed differences in defect density across different forms. The characteristic D, G, and D' bands varied in relative intensity, offering insight into structural integrity and functionalization effects. XPS measurements examined core-level spectra (C 1s, F 1s, N 1s), revealing chemical bonding environments and hybridization states, including the sp^2 and sp^3 states. A notable decline in fluorine content in F-graphene suspensions and inks, relative to powders, was observed. Existence of organic fluorine and total absence of metallic fluorine were observed. Raman spectroscopy and XPS data provided a correlated view of structural and chemical evolution through the graphene production chain (Figure 1).

[1] M. Zhang et al., Mater. Chem. Front., 1, 37–60 (2017)

[2] A. J. Pollard et al., NPL, Good Practice Guide No. 145 (2017)

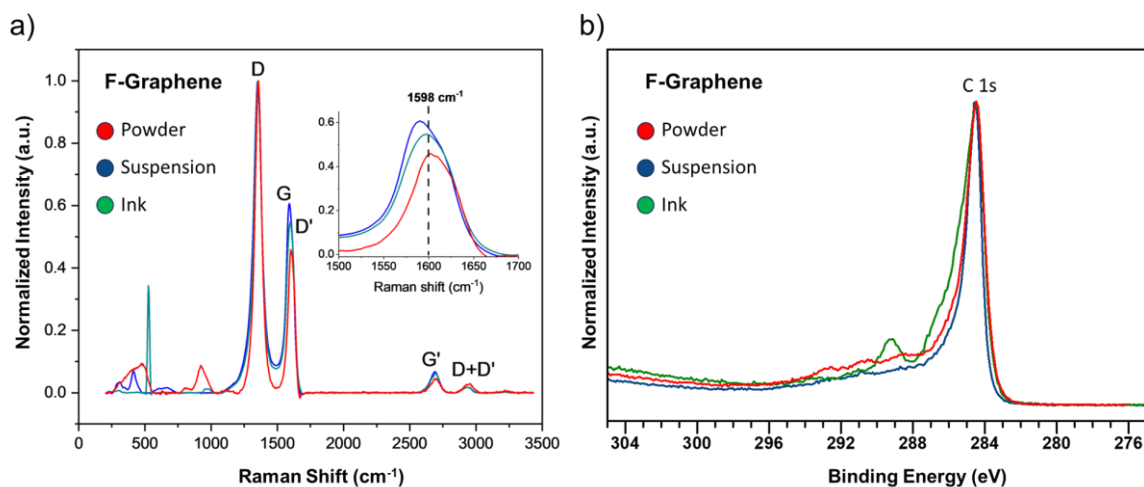


Figure 1: a) Raman spectra and b) high-resolution XPS for C 1s for the F-functionalized material as powder, in suspension and embedded in ink.