Chemical functionalization and characterization of hexagonal Boron Nitride nanosheets

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Hexagonal Boron Nitride (hBN) is a wide band gap insulator with high thermal stability, and widely used in lubricants, protective coatings, and polymeric composites. Due to its chemical inertness, the surface functionalization of hBN is challenging. Here, we propose an effective one step process able to exfoliate and activate the hBN nanosheets to be amenable to covalent functionalization. We intercalate K into bulk hBN powder followed by its exfoliation as negatively charged single and few-layer hBN nanosheets in tetrahydrofuran (THF) under an inert environment. The resulting chemically activated negatively charged hBN nanosheets react with alkyl halides, resulting in functionalized (alkylated) hBN nanosheets. The alkylated hBN nanosheets were characterized by Thermogravimetric Mass Spectrometry (TG-MS), Fourier transformed infra -red spectroscopy (FT-IR), Ultraviolet – visible spectroscopy (UV-Vis) and High-Resolution Transmission Electron Microscopy (HR-TEM). For the alkylated hBN nanosheet samples, XPS data showed an increase in carbon content, compared to the control. When heated under an inert N_2 environment, TG analysis showed a weight loss of up to 5 % in the functionalized samples, which correspond to the detachment of the alkyl sidechains from the hBN nanosheets. This was confirmed by MS analysis, which detected mass traces of alkyl chain fragments at *m/z* 41(C_3H_5), 43 (C_3H_7), and 55 (C_4H_7). When dispersed in non-polar solvents such as benzene, the functionalized 2D hBN nanosheets showed stable dispersions when compared to pristine samples. This improved dispersibility is expected to unlock the full potential of hBN in many applications including nanocomposite materials, printable inks, and sensors.