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## Material Science 2020: A Novel Mechano-Chemical Synthesis Route for Fluorination of Hexagonal Boron Nitride Nanosheets - Agrabul Ahmad- Dalian University of Technology, China

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## Abstract

This paper presents a facile, two-step mechano-chemical route to exfoliate and fluorinate hexagonal boron nitride nanosheets (BNNSs). The influence of fluorine (F) chemisorption on the optical and magnetic properties of BNNSs is investigated. It has been observed experimentally, by increasing fluorine concentration, band gap lowers from ~5to4.17 eV and saturation magnetization and coercivity achieves the value of 1.8322x10-3 emu/g and 157.25Oe, respectively. Furthermore, results strongly supported that during synthesis there is a direct correlation between different number of few atomic layers and adsorption of fluorine atoms towards fluorination of BNNSs. Moreover the defective boron sites are thermodynamically most stable and favorable for fluorine adsorption to form stable B-F bonds as compared to N-F bonds. Such observations are additionally supported by theoretical calculations considering various possible fluorine-based defects in h-BN nanostructure. Hence, a narrow optical band gap with a room temperature weak ferromagnetic diluted magnetic semiconducting behavior of BNNSs via fluorination will expand their usage in designing/fabricating magnetic, electronic and nano-devices. Keywords: BNNSs; exfoliation; ball milling; fluorination and band gap calculation.

## **Recent Publications:**

- Agrab ul Ahmad, Hongwei Liang ,Qasim Abbas etc. A novel mechano-chemical synthesis route for fluorination of hexagonal boron nitride nanosheets. Impact factor 3.5
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