

## Scrutinizing XAFS spectroscopy and biocompatibility of N-doped edge-functionalized graphene oxide

Gopal Avashthi<sup>1</sup>, Shrikant S. Maktedar<sup>1</sup>, Man Singh<sup>1</sup><sup>1</sup>School of Chemical Sciences, Central University Of Gujarat, Gandhinagar, India

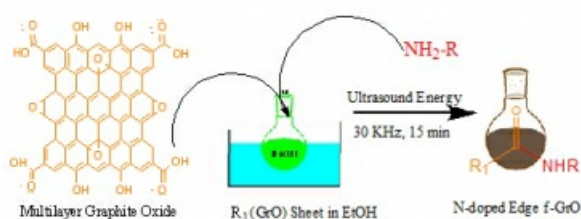
E-mail: gopalavashthi@gmail.com

The synthesis of the Graphite Oxide and its composites is explored for the various advanced applications like ORR, OER, HER, photocatalyst and supercapacitor performance. But the biological aspects are an interesting study for the cytotoxicity profile. The sonochemical assisted exfoliation of the graphite oxide leading to exfoliate into the single layer graphene oxide (GrO). Here, mechanochemical energy employed for the breaking the Van der Waal's forces between the layers and helping to enhanced the reactivity of the local electronic environment towards the edge of GrO. The ultrasound assisted synthesis of the N-doped edge-functionalized graphene oxide (f-GrO) with the various amine substituted heterocyclic moieties through nucleophilic substitution reaction via in-situ esterification mechanism, skips the complete deletion of the hazardous and acylating coupling reagents. The synergistic impact of N-doped edge f-GrO is noticed as the changed the crystalline behaviour, surface morphology and biocompatibility. However, the crystalline behaviour of N-doped edge f-GrO was confirmed with HRTEM-SAED patterns, Raman and XRD. The enhanced thermal stability of the N-doped edge f-GrO demonstrates by the thermal gravimetric analysis (TGA). The involvement of the amine substituted moieties toward the edge as N-doped confirmed with the X-ray absorption fine structure spectroscopy (XAFS) plot with evolved electronic transitions between the absorption coefficients as a function of photon energy. The higher energetic unoccupied  $\sigma^*$  and  $n^*$  states have confirmed, the role of C\_K edges towards edge functionalization. The comparative analysis of the consecutive N-doped edge f-GrO show distinct % degree of affinity towards the edge. Thus the local electronic environments of an atom in successive N-doped edge f-GrO have characteristics intense peaks. The XAFS of GrO and N-doped f-GrO shows that the newly evolved electronic state between pre and post edge with change intensity at C\_K Edge. Similarly, the N-doped edge f-GrO was explored at C\_K edge, O\_K edge, and N\_K edge for the validation of the N-doping. The intensity appears with new electronic state in the C\_K edge and O\_K edge at 288.1 eV and 530.07 eV respectively. The sharp edge structure at O\_K edge resolute the impact of electronic transition from  $n$  to  $\sigma^*$  state of OH. However, the sharp and intense spectra of XAFS analysis near N\_K edge at 400 eV, confirmed the N-doping with GrO. The presence of the oxygen functionality at edge of GrO, shows difficulties in transition of electron from nonbonding energy level ( $n$ ) to higher antibonding energy level ( $\sigma^*$ ). N-doping causes easy  $n$  to  $\sigma^*$  electronic transition due to removal of oxygen moieties from the edge. Therefore the N-doped edge f-GrO observed with sharp and intense peak of XAFS spectroscopy analysis as compared to the GrO and Gt. The biocompatibility study of N-doped edge f-GrO was explored with in vitro assessment on Vero living cell line with sulforhodamine B (SRB) assay at 10, 20, 40 and 80  $\mu\text{g mL}^{-1}$  more than 80%. The morphological impact of N-doped edge f-GrO on Vero cell line clearly supports the synthesis of biocompatible graphene based N-doped composite materials.

[1] Gandhiraman, R. P. et al. (2014). J. Phys. Chem. C, 118, 18706–18712.

[2] Wang, Y. F. et al. (2015). Sci. Rep. 5, 15439-12.

[3] Zhan, D. et al. (2011). Carbon, 49, 1362-1366.



**Keywords:** [X-ray absorption fine structure spectroscopy](#), [biocompatibility](#), [N\\_K edge](#)