

*Supporting Information*

# Superior X-ray Radiation Shielding Effectiveness of Biocompatible Polyaniline Reinforced with Hybrid Graphene Oxide-Iron Tungsten Nitride Flakes

Seyyed Alireza Hashemi <sup>1,2,\*</sup>, Seyyed Mojtaba Mousavi <sup>3,2</sup>, Reza Faghihi <sup>4,5</sup>, Mohammad Arjmand <sup>6</sup>, Mansour Rahsepar <sup>7</sup>, Sonia Bahrani <sup>2</sup>, Seeram Ramakrishna <sup>1</sup>, and Chin Wei Lai <sup>8</sup>

<sup>1</sup> Department of Mechanical Engineering, Center for Nanofibers and Nanotechnology, National University of Singapore, Singapore; [seeram@nus.edu.sg](mailto:seeram@nus.edu.sg)

<sup>2</sup> Department of Medical Nanotechnology, School of Advanced Medical Sciences and Technologies, Shiraz University of Medical Sciences, Shiraz, Iran; [kmepo.smm@gmail.com](mailto:kmepo.smm@gmail.com) (S.M.M.); [s.bahrani22@gmail.com](mailto:s.bahrani22@gmail.com) (S.B.)

<sup>3</sup> Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan

<sup>4</sup> Nuclear Engineering Department, Shiraz University, Shiraz, Iran. 71936-16548; [faghihir@shirazu.ac.ir](mailto:faghihir@shirazu.ac.ir)

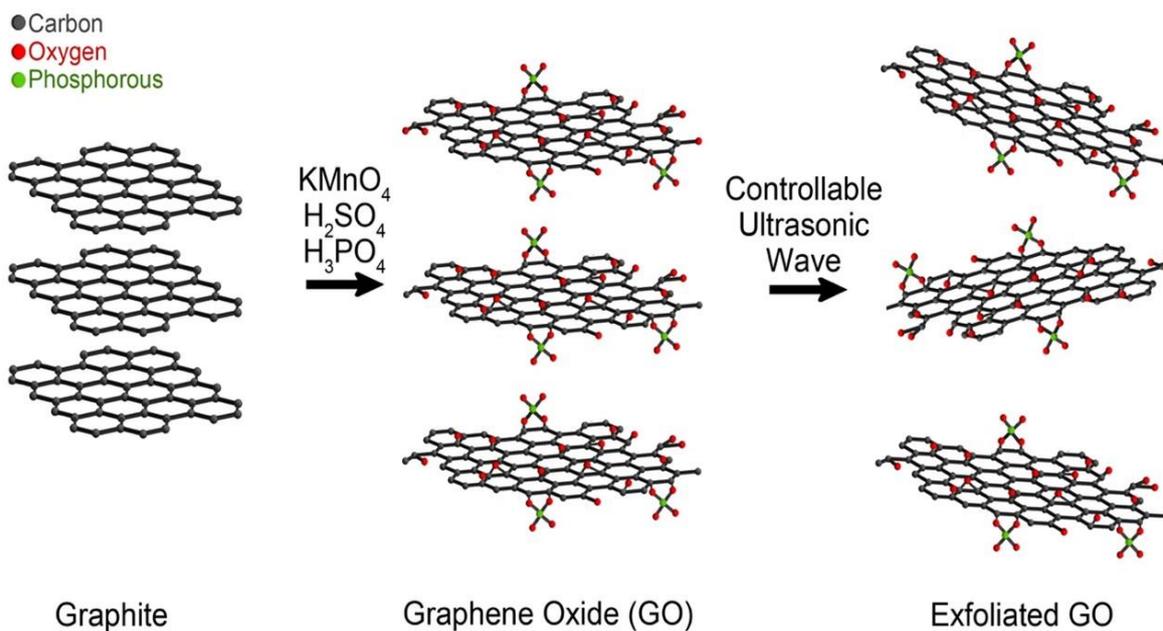
<sup>5</sup> Radiation Research Center, Shiraz University, Shiraz, Iran. 71936-16548

<sup>6</sup> School of Engineering, University of British Columbia, Kelowna, BC, V1V 1V7, Canada; [mohammad.arjmand@ubc.ca](mailto:mohammad.arjmand@ubc.ca)

<sup>7</sup> Department of Materials Science and Engineering, School of Engineering, Shiraz University, Zand Boulevard, Shiraz, Iran. 71348-51154; [mansour.rahsepar@gmail.com](mailto:mansour.rahsepar@gmail.com)

<sup>8</sup> Nanotechnology & Catalysis Research Center, University of Malaya, Malaysia; [cwlai@um.edu.my](mailto:cwlai@um.edu.my)

\* Correspondence: [sa\\_hashemi@sums.ac.ir](mailto:sa_hashemi@sums.ac.ir) (S.A.H.); Tel: 0098 9398432509



**Figure S1.** Formation of GO out of pure graphite flakes.

**Table S1.** Specification of developed samples.

Sample Number	GO-ITN (wt%)	Thickness (mm)	Diameter (cm)
1	0	0.95	2
2	0	1.2	2
3	25	0.95	2
4	25	1.2	2
5	50	0.95	2
6	50	1.2	2

**Table S2.**  $I_D/I_G$  ratio obtained by current method compared with literature.

**Table S3.**

Production method	Type of Graphene	I <sub>D</sub> /I <sub>G</sub>	Ref.
Hummers	rGO	0.88 - 0.92	[1]
Hummers	GO	1.14 - 1.19	[2]
Hummers	rGO	1.28 - 2.70	[2]
Modified Hummers	GO	1.42 - 1.88	[3]
Modified Hummers	rGO	1.12 - 1.24	[3]
Modified Hummers	GO	0.97	[4]
Modified Hummers	rGO	1.15 - 1.4	[4]
Modified Hummers	GO	1.07	[5]
Current study	GO	0.835	-

Element analysis of fabricated GO via XPS.

Name	Peak BE	FWHM eV	Area (p) CPS.eV	Atomic %
C1s	284.72	1.65	57958.50	68.36
O1s	532.65	2.07	63486.40	31.00
N1s	401.05	0.94	850.10	0.65

**Table S4.** De-convolution of peak C1s into five diverse segments.

Peak / eV	FWHM eV	Area (p) CPS.eV	Atomic %
Sp <sup>1</sup> (283.78 eV)	1.65	1902.42	3.33
Sp <sup>2</sup> (284.78 eV)	1.48	23762.61	41.62
Sp <sup>3</sup> (286.85 eV)	1.35	21682.91	38.03
C=O (288.61 eV)	1.74	8006.78	14.06
O-C=O (290.48 eV)	2.17	1682.09	2.96

**Table S5.** De-convolution of peak N1s into three diverse segments.

Peak / eV	FWHM eV	Area (p) CPS.eV	Atomic %
Pyridinic Nitrogen (397.33 eV)	1.92	127.18	19.87
Pyrrolic Nitrogen (400.19 eV)	1.92	260.53	40.79
Pryidine-N-Oxide (402.08 eV)	1.92	251.00	39.35

**Table S6.** De-convolution of peak O1s into four diverse segments.

Peak / eV	FWHM eV	Area (p) CPS.eV	Atomic %
C=O (531.47 eV)	1.54	11234.61	18.08
C-OH (532.66 eV)	1.54	39625.13	63.83

C-O (533.74 eV)	1.54	8335.48	13.44
C-OH (535.53 eV)	1.92	2877.73	4.65

**Table S7.** XPS and XRD results comparison between previous methods and current study.

Method	Type of graphene	sp <sup>1</sup> hybridization (%)	sp <sup>2</sup> hybridization (%)	sp <sup>3</sup> hybridization (%)	d-spacing (Å)	Ref.
Hummer	GO	-	39	61	8	[6]
Hummer	rGO	14.6	67.8	17.6	8.133	[7]
Modified Hummer	GO	-	37	63	9	[6]
Modified Hummer	GO	35	-	65	9.06	[8]
Improved Method	GO	-	31	69	9.5	[6]
Hofmann	rGO	14.2	67.1	18.7	7.226	[7]
Staudenmaier	rGO	13.2	69.3	17.5	7.084	[7]
Current study	GO	3.3	41.6	55.1	3.8499	-

**Table S8.** EDAX analysis of hybrid GO-ITN flakes.

Element	Intensity	Weight %	Atomic %
C	17.9	8.02	31.26
N	3.1	1.87	6.26
O	64.8	11.87	34.74
Fe	352.3	13.39	11.23
W	247.5	64.85	16.52

**Table S9.** Specification of appeared peaks of iron tungsten nitride's structure.

Position (2 $\theta$ )	d-spacing (Å)	(h k l)	Chemical formula	Crystalline size (Å)	Micro strain (%)
27.9181	3.19588	(2 2 2)	W <sub>96</sub> Fe <sub>40</sub> N <sub>8</sub>	157.2079	1.01645
32.3874	2.76435	(0 0 4)	W <sub>96</sub> Fe <sub>40</sub> N <sub>8</sub>	392.3921	0.352243
46.3768	1.95791	(0 4 4)	W <sub>96</sub> Fe <sub>40</sub> N <sub>8</sub>	337.9722	0.289655

Peaks were extracted from reference number 96-200-6776 related to the iron tungsten nitride (i.e., W<sub>96</sub>Fe<sub>40</sub>N<sub>8</sub>) that exhibit cubic structure and its crystalline specifications are as follow: a (Å): 11.11, b (Å): 11.11, c (Å): 11.11, alpha (°): 90, beta (°): 90, gamma (°): 90, calculated density: 24.21 g.cm<sup>-3</sup> and volume of cells 1371.33 × 10<sup>6</sup> pm<sup>3</sup>.

**Table S10.** Performance of the developed shields against incident X-ray waves.

Sample	Detected X-ray (μGy)			Attenuated X-ray (μGy)			X-ray Absorption (%)		
	30 kV	40 kV	60kV	30 kV	40 kV	60kV	30 kV	40 kV	60kV
<b>Control</b>	141.2	1003	2178	-	-	-	-	-	-
<b>1</b>	123.9	912.3	2037	17.3	90.7	141	12.252	9.0428	6.473
<b>2</b>	121.4	900.8	2015	19.8	102.2	163	14.022	10.189	7.483
<b>3</b>	72.14	678.6	1717	69.06	324.4	461	48.909	32.342	21.166
<b>4</b>	55.71	584.9	1566	85.49	418.1	612	60.545	41.684	28.099
<b>5</b>	38.98	481.01	1372	102.22	521.99	806	72.393	52.042	37.006
<b>6</b>	30.96	430	1198	110.24	573	980	78.073	57.128	44.995

**References:**

- Gupta, B.; Kumar, N.; Panda, K.; Kanan, V.; Joshi, S.; Visoly-Fisher, I. Role of oxygen functional groups in reduced graphene oxide for lubrication. *Scientific Reports* **2017**, *7*, 45030.
- Eigler, S.; Dotzer, C.; Hirsch, A. Visualization of defect densities in reduced graphene oxide. *Carbon* **2012**, *50*, 3666-3673.
- King, A.A.; Davies, B.R.; Noorbehesht, N.; Newman, P.; Church, T.L.; Harris, A.T.; Razal, J.M.; Minett, A.I. A New Raman Metric for the Characterisation of Graphene oxide and its Derivatives. *Scientific reports* **2016**, *6*.
- Rajagopalan, B.; Chung, J.S. Reduced chemically modified graphene oxide for supercapacitor electrode. *Nanoscale research letters* **2014**, *9*, 535.
- Gupta, V.; Sharma, N.; Singh, U.; Arif, M.; Singh, A. Synthesis and characterization of Graphene Oxide. *Optik-International Journal for Light and Electron Optics* **2017**.
- Marcano, D.C.; Kosynkin, D.V.; Berlin, J.M.; Sinitskii, A.; Sun, Z.; Slesarev, A.; Alemany, L.B.; Lu, W.; Tour, J.M. Improved synthesis of graphene oxide. **2010**.
- Poh, H.L.; Šaněk, F.; Ambrosi, A.; Zhao, G.; Sofer, Z.; Pumera, M. Graphenes prepared by Staudenmaier, Hofmann and Hummers methods with consequent thermal exfoliation exhibit very different electrochemical properties. *Nanoscale* **2012**, *4*, 3515-3522.
- Tao, C.-a.; Wang, J.; Qin, S.; Lv, Y.; Long, Y.; Zhu, H.; Jiang, Z. Fabrication of pH-sensitive graphene oxide-drug supramolecular hydrogels as controlled release systems. *Journal of Materials Chemistry* **2012**, *22*, 24856-24861.