

## **Supporting Information**

# **Understanding the Endocrine Disruptor and Determination of Bisphenol A by Functional Cu-BTABB- MOF/rGO Composite as Facile Rapid Electrochemical Sensor: An Experimental and DFT Investigation**

**Srikanth Ponnada<sup>[a,f]\*</sup>, Demudu Babu Gorle<sup>[b]</sup>, Maryam Sadat Kiai<sup>[c]</sup>, Chikkili Venkateswara  
Raju<sup>[d]</sup>, Mehrdad Faraji<sup>[e]</sup>, Rakesh K Sharma<sup>[f]\*</sup> & Annapurna Nowduri<sup>[a]\*</sup>**

*<sup>a</sup>Department of Engineering Chemistry, Andhra University College of Engineering (A), Andhra University, Visakhapatnam-530003, India.*

*<sup>b</sup>Materials Research Centre, Indian Institute of Science, Bangalore-560012, India.*

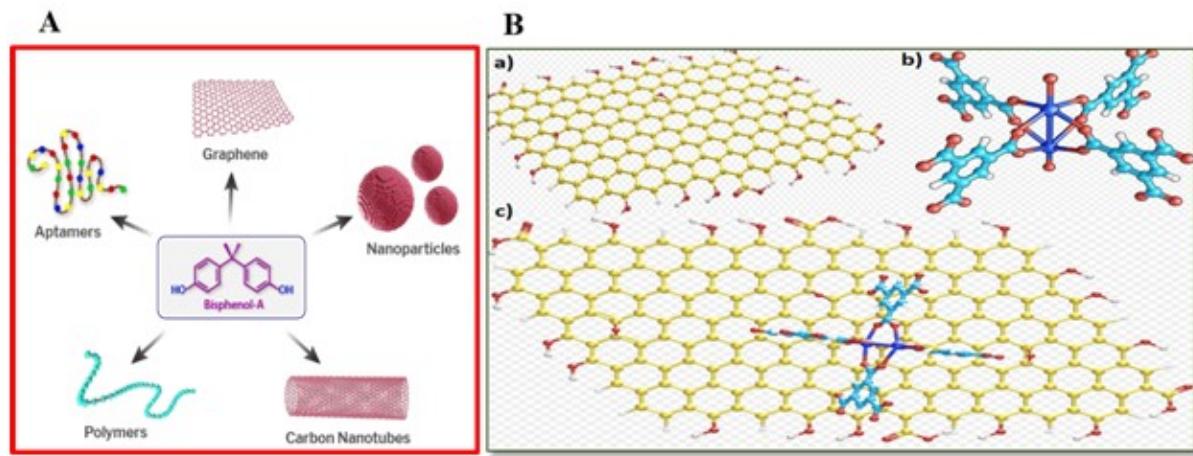
*<sup>c</sup>Nano-Science and Nano-Engineering Program, Graduate School of Science, Engineering and Technology, Istanbul Technical University, Istanbul-34469, Turkey.*

*<sup>d</sup>Research Center for Photoenergy Harvesting & Conversion Technology (phct), Department of Energy Materials and Engineering, Dongguk University, Seoul, 04620, Republic of Korea.*

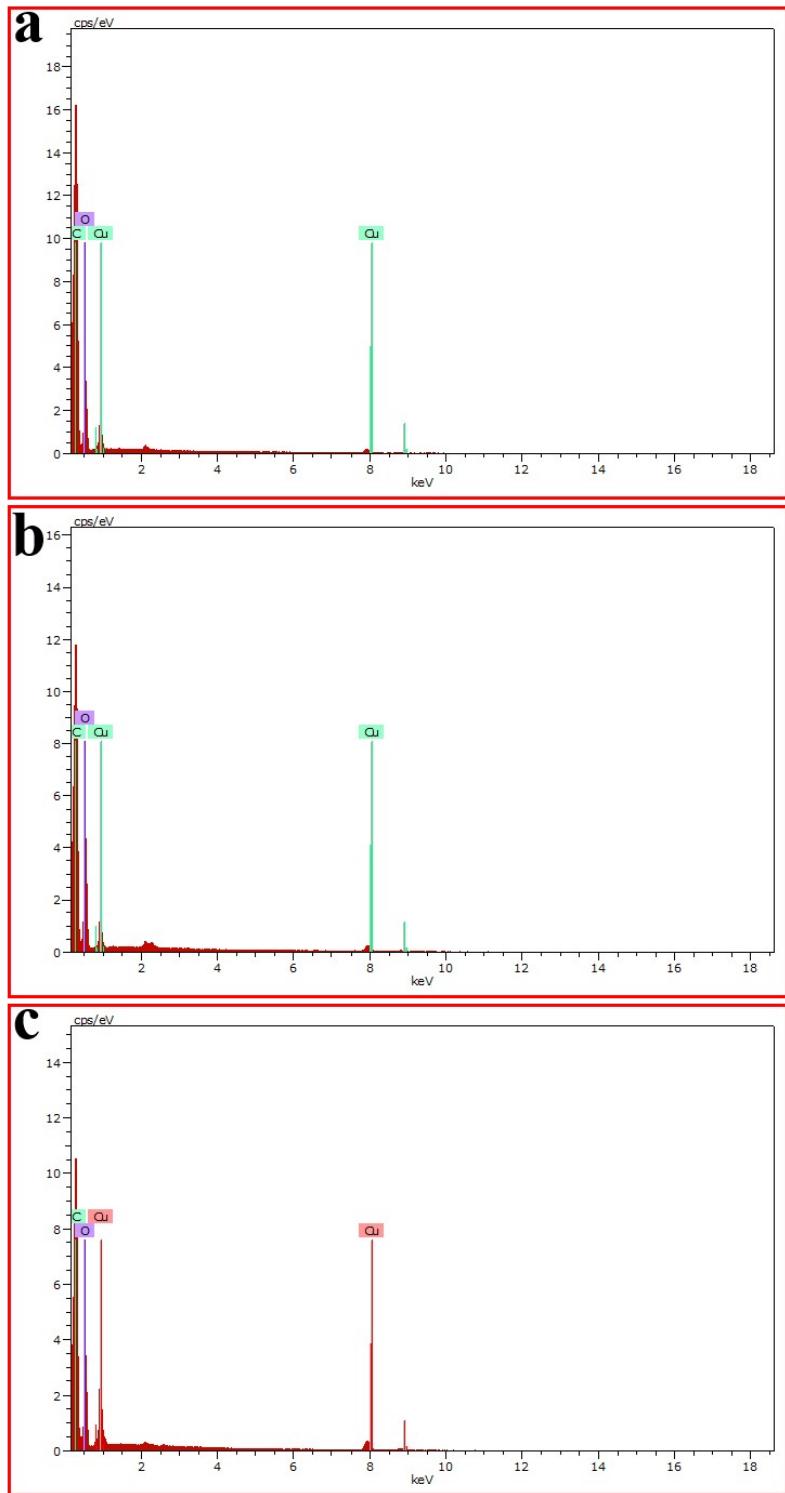
*<sup>e</sup>Department of Micro and Nanotechnology, Graduate School of Science and Engineering, TOBB University of Economics and Technology, Ankara-06530, Turkey.*

*<sup>f</sup>Sustainable Materials and Catalysis Research Laboratory (SMCRL), Department of Chemistry, Indian Institute of Technology Jodhpur, Karwad, Jodhpur-342037, India.*

**Corresponding authors:** [dr.nannapurna@andhrauniversity.edu.in](mailto:dr.nannapurna@andhrauniversity.edu.in)  
[rks@iitj.ac.in](mailto:rks@iitj.ac.in)  
[koolsreekanth@gmail.com](mailto:koolsreekanth@gmail.com)



**Figure S1.** (A). Bisphenol-A analysis sensors. (B). Representation of the electrochemical interaction of MOF and Cu-BTABB-MOF on GO and rGO. (a) r-GO, (b)Cu-BTABB-MOF,(c) Cu-BTABB-MOF@ r-GO. Red, Yellow, Gray and Blue colors are Oxygen, Hydrogen, Carbon and Nitrogen, respectively.



**Figure S2.** EDX spectra of (a) Cu BTABB-MOF, (B) Cu BTABB-MOF/GO, and (c) Cu BTABB-MOF/rGO.

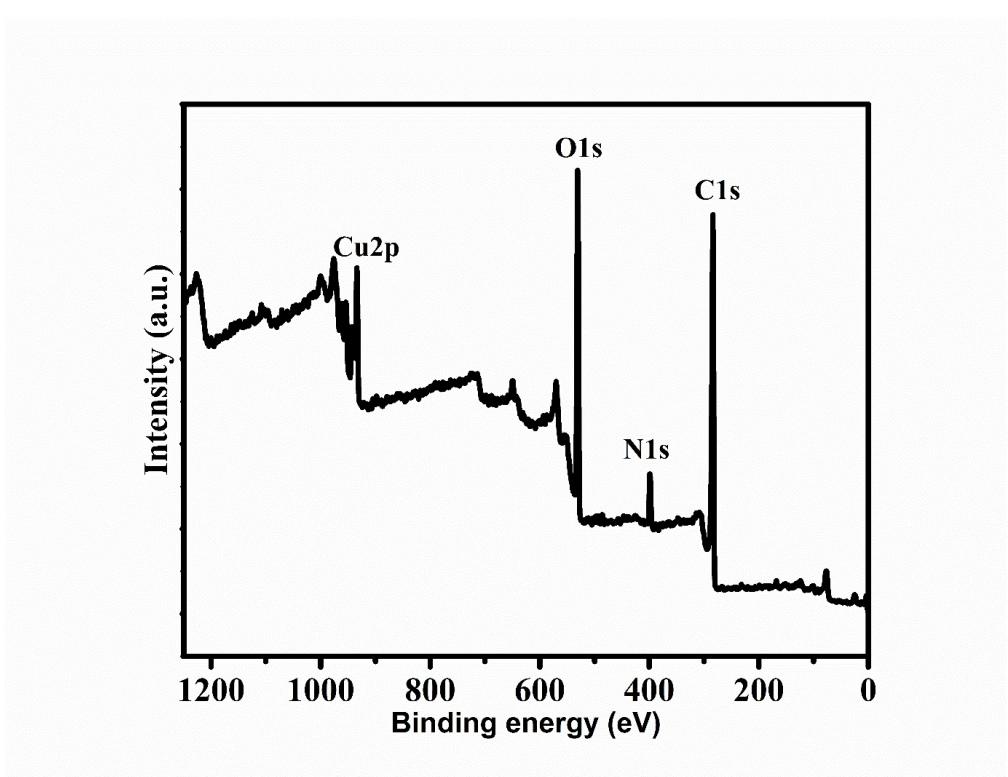


Figure S3. XPS survey spectra of Cu BTABB-MOF/rGO.

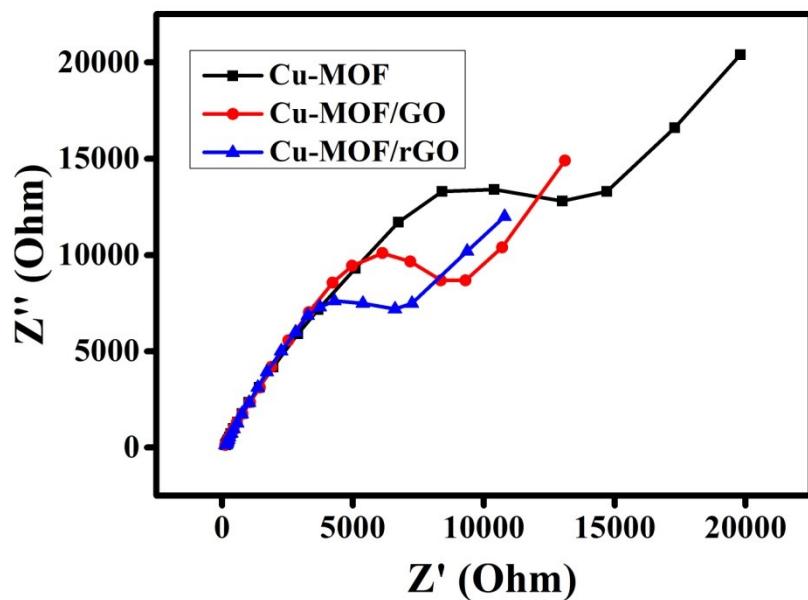
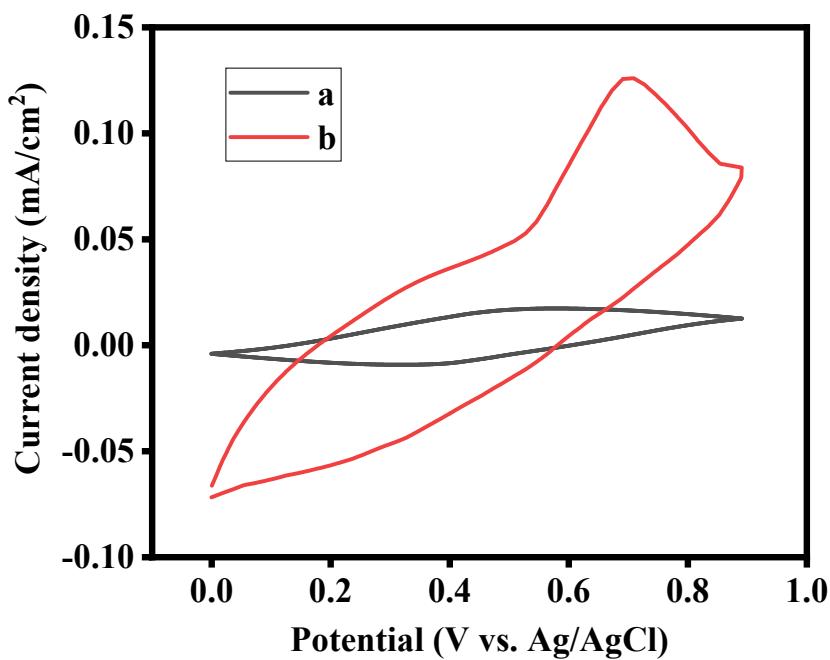
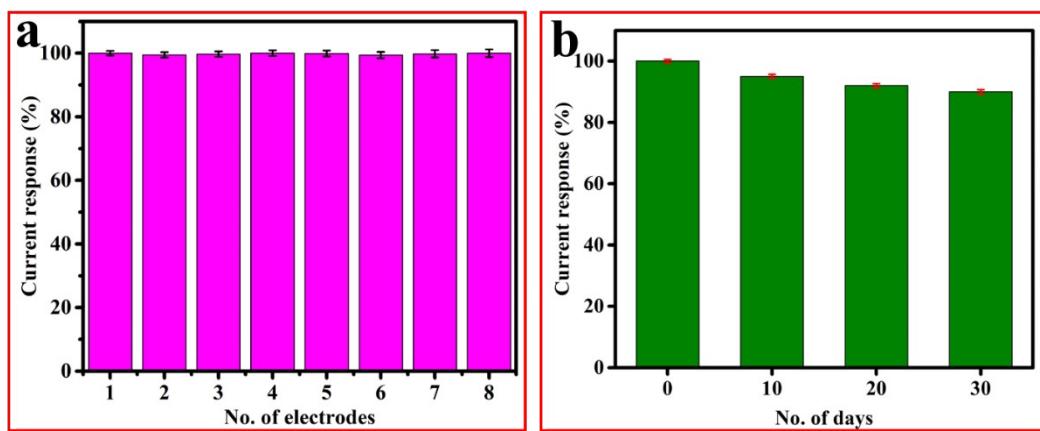


Figure S4. EIS of Cu-MOF, Cu-MOF/GO and Cu-MOF/rGO.



**Figure S5.** CV of Cu-MOF/rGO in the absence (a) and presence (b) of 100  $\mu\text{M}$  BPA in 0.1 M PBS (pH 7.4) at 50 mV/s.



**Figure S6.** (a) Reproducibility study of Cu-BTABB-MOF@rGO on eight different electrodes and its current response, (b) Stability study of Cu-BTABB-MOF@rGO with 10 'days' time interval up to 30 days.

**Table S1.** Rate of recovery % and RSD % of real time analysis

Sample	BPA added ( $\mu\text{M}$ )	Found ( $\mu\text{M}$ )	Recovery (%)	RSD%
Water sample 1	1	1.057	105.7	2.7 3.1 2.8
Water sample 2	5	5.043	100.86	
Water sample 3	10	10.082	100.82	

Tab  
leS2

.Comparison of the Present Cu BTABB-MOF/rGO Fabricated Sensor with the Reported Sensors  
 Towards Electrochemical Sensing of Bisphenol A

Modified electrode	Analyte	Linear Range	LOD	References
MWCNTs / $\beta$ -cyclodextrin ( $\beta$ CD)	BPA	0.125 - 2 and 2 - 30 $\mu\text{M}$	13.76 nM	S1
Polyglutamic acid/amino-functionalized carbon nanotubes nanocomposite	BPA	0.1-10 $\mu\text{M}$	0.02	S2
Magnetic molecularly imprinted polymer (USMagMIP)/ nanocomposite of carbon black nanoparticles (CBNPs/ Gold nanoparticles (AuNPs)	BPA	0.07-10 $\mu\text{M}$	8.8 nM and 31.5 nM	S3
Platinum nanoparticles (DPNs) / gold nanoparticles / polyethyleneimine-phosphatidylcholine (PEI-PC) layer	BPA	0.01-1.0 and 1.0-300 $\mu\text{M}$	6.63 $\pm$ 0.77 nM	S4
Cerium/centered metal-organic framework / reduced graphene oxide composite (Ce-MOF-ERGO)	BPA	3 nM-10 $\mu\text{M}$	1.9 nM	S5
Ni/MOF@CNTs	BPA	0.001-1.0 $\mu\text{M}$	0.35 nM	S6
Ionic liquid functionalized graphene nanoplatelets	BPA	0.02-5.0 $\mu\text{M}$	6.4 $\mu\text{M}$	S7

Copper-centered metal-organic framework (MOF)	BPA	0.05-3.0μM	0.013 μM	<b>S8</b>
Amine-functionalized MOF/reduced graphene oxide composites	BPA	2-200 μM	0.7966 μM	<b>S9</b>
Covalent organic framework CTpPa-2	BPA	0.1-50μM	0.02 μM	<b>S10</b>
<b>Cu BTABB-MOF/rGO</b>	<b>BPA</b>	<b>0-10μM</b>	<b>0.2μM</b>	<b>This work</b>

## References

- [S1] M. Y. Ali, A. U. Alam and M. M. R. Howlader, *Sens. Actuators B: Chem.*, 2020, **320**, 128319.
- [S2] Y. Lin, K. Liu, C. Liu, L. Yin, Q. Kang, L. Li and B. Li, *Electrochim. Acta*, 2014, **133**, 492-500.
- [S3] N. B. Messaoud, A. A. Lahcen, C. Dridi and A. Amine, *Sens. Actuators B: Chem.*, 2018, **276**, 304-312.
- [S4] K. Shim, J. Kim, M. Shahabuddin, Y. Yamauchi, M. S. A. Hossain and J. H. Kim, *Sens. Actuators B: Chem.*, 2018, **255**, 2800-2808.
- [S5] X. Wang, Y. Shi, J. Shan, H. Zhou and M. Li, *Ionics*, 2020, **26**, 3135-3146.
- [S6] C. Xu, L. Liu, C. Wu and K. Wu, *Sens. Actuators B: Chem.*, 2020, **310**, 127885.
- [S7] P. Butmee, P., G. Tumcharern, P. Saejueng, D. Stankovic, A. Ortner, J. Jitcharoen, K. Kalcher and A. Samphao, *J. Electroanal. Chem.*, 2019, **833**, 370-379.
- [S8] X. Wang, X. Lu, L. Wu and J. Chen, *Biosens. Bioelectron.*, 2015, **65**, 295-301.
- [S9] J. Cheng, S. Chen, D. Chen, L. Dong, J. Wang, T. Zhang, T. Jiao, B. Liu, H. Wang, J. -J. Kai, D. Zhang, G. Zheng, L. Zhi, F. Kang and W. Zhang, *J. Mater. Chem. A*, 2018, **6**, 20254-20266.

**[S10]** Y. -H. Pang, Y. -Y. Huang, L. Wang, X. -F. Shen and Y. -Y. Wang, *Environ. Pollut.*, 2020, **263**, 114616.