

Supporting information

Aluminium MOF as a Selective Sensor for Atrazine with Docking and Computational Insight

Simranjeet Singh¹, Radhika Varshney^{1#}, Pavithra N^{1#}, Basavaraju Uppara^{2,3}, Praveen C Ramamurthy^{1*}, Nabila Shehata^{4,5}

¹Interdisciplinary Centre for Water Research (ICWaR), Indian Institute of Science, Bengaluru, Karnataka 560012, India

²Department of Materials Engineering, Indian Institute of Science, Bengaluru, Karnataka 560012, India

³Centre for Smart Manufacturing Precision Machine Tools & Aggregates (C-SMPM), Central Manufacturing Technology Institute (CMTI), Bengaluru, Karnataka 560022, India

⁴Environmental Science and Industrial Development Department, Faculty of Postgraduate Studies for Advanced Sciences, Beni-Suef University, Egypt

⁵Renewable Energy Department, Korean Egyptian Faculty for Industry and Energy Technology, Beni-Suef Technological University

*Corresponding author: praveen@iisc.ac.in

3.3 Electrochemical characterization using CV and EIS:

The cyclic voltammograms of the bare carbon paste electrode (BCPE) and the modified carbon paste electrode (MCPE) have been performed in 0.1 M HCl buffer (**Figure S1a**). The MCPE exhibits a significantly higher current response compared to the BCPE over the entire potential range, indicating enhanced electrochemical activity. The increased peak currents observed for the MCPE suggest improved electron transfer kinetics and higher conductivity due to the surface modification. These results demonstrate that the MCPE offers superior electrochemical performance, making it a promising platform for sensing applications.

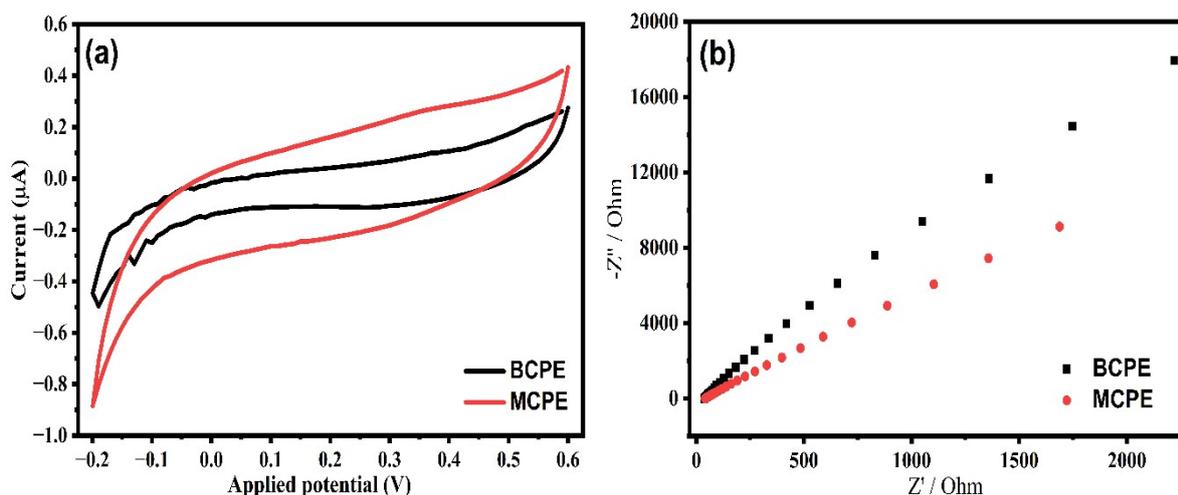


Figure S1: a) Cyclic voltammograms of BCPE and MCPE in 0.1 N HCl, b) Nyquist plot of Al-MOF with atrazine in 0.1 N HCl.

The Nyquist plot of the BCPE and the MCPE is presented in **Figure S1b**. The plot depicts the imaginary component of impedance ($-Z''$) versus the real component (Z') and reveals distinct electrochemical behaviours for the two electrodes. The BCPE exhibits a higher overall impedance, with $-Z''$ values reaching approximately 17,000 Ω , whereas the MCPE shows a significantly lower impedance, with a maximum $-Z''$ of around 9,000 Ω . This reduction in impedance upon modification indicates enhanced charge transfer and improved electrochemical kinetics at the electrode surface. The results clearly demonstrate that electrode modification effectively facilitates electron transfer, making MCPE a more efficient platform for electrochemical applications.

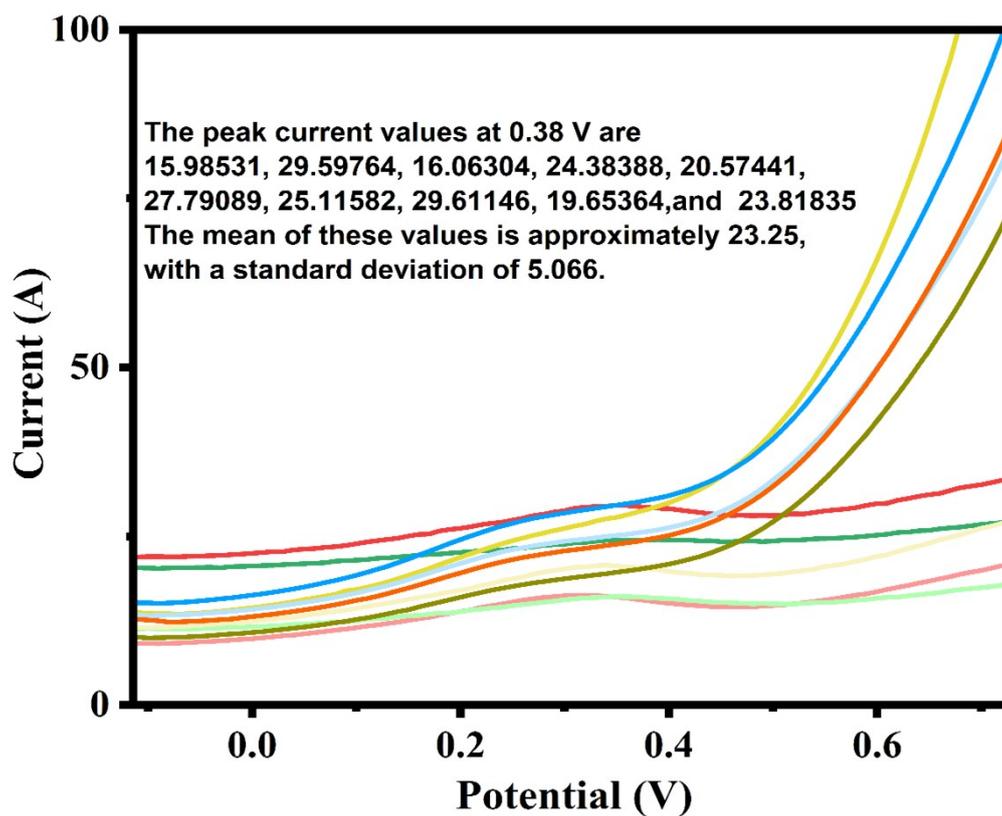


Figure S2: Blank DPV curves along with the standard deviation calculation for Blank samples

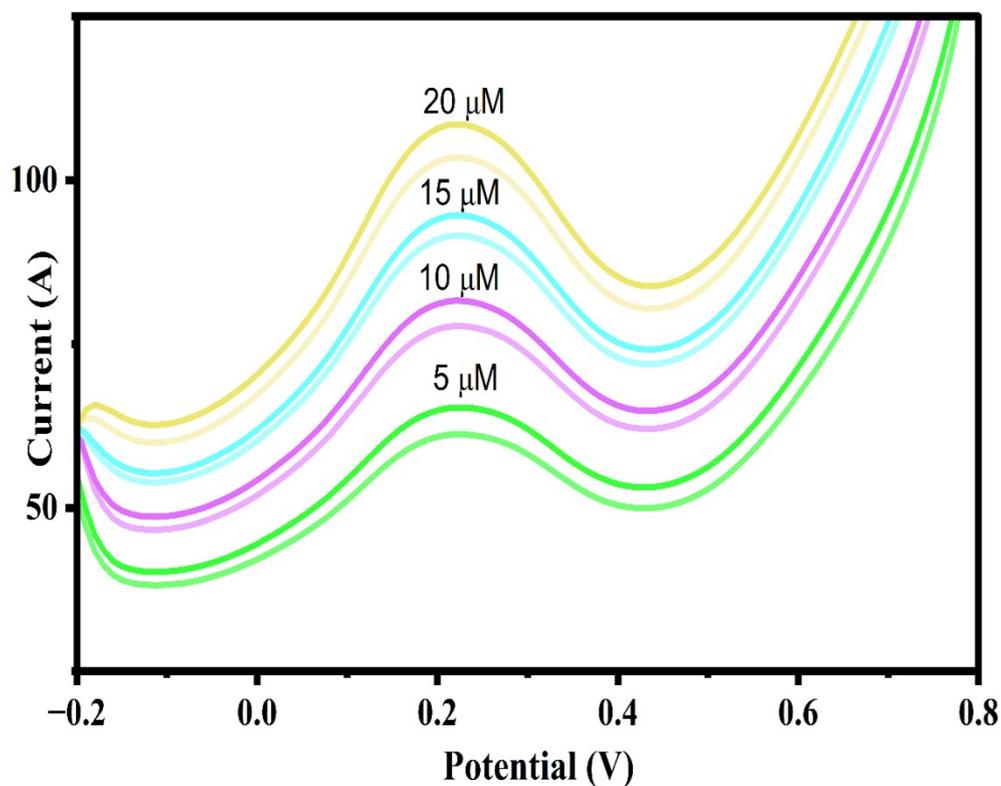


Figure S3: Duplicate runs for the deionised water samples spiked with atrazine in 0.1 N HCl buffer.