

Supplementary information

Ni-Fe Layered Double Oxide on Porous Nickel Foam: A Rationalized Approach to Electrochemical Sensing of Atrazine Herbicide in Water Samples

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1. Choice of material

Among the different types of transition metal-based LDHs, Ni²⁺-Fe³⁺ LDH is affirmed as an ideal electroactive material because of its higher electro-catalytic activity outperforming most of the known hydroxides. The excellent catalytic activity of Ni-Fe LDH can be attributed to its higher number of coordination sites at the edges along with the enhanced redox activity of Ni and Fe creating high valence materials. The oxidation of Ni²⁺ to NiOOH species is facilitated by the coexistence of Fe³⁺, thereby modulating the electronic structure via partial charge transfer. The Fe species existing at the edge sites can also positively alter the catalytic action of Ni²⁺. In addition to this, high earth abundance, environmental benignity, and reasonable cost are the other significant contributing aspects toward its utilization. The integration of CO₃²⁻ ions as the charge-balancing species within the interlayers results in faster intercalation because of their increased affinity as compared to other inorganic anions.

2. Effect of pH

Supporting electrolyte plays a significant role in the electrochemical analysis as it affects the kinetics, charge transfer and stability of the electrode. Here the influence of different buffer systems was monitored and finally NaOH was fixed as the electrolyte for every study. Further the effect of pH of the electrolyte was monitored from 6 to 12 in the presence of 0.01mM ATZ. Better peak separation and current response were observed at pH 10, therefore every study was conducted at this pH. In an alkaline medium, the concentration of hydroxide ions (OH^-) is higher compared to acidic or neutral solutions. The increase in hydroxide ion concentration affects the chemical reactivity and equilibrium of reactions occurring in the alkaline medium. In higher pH solutions, solubility of ATZ is also high. The alkaline conditions at pH 10 can promote various chemical transformations of atrazine. For example, it can undergo nucleophilic substitution reactions or ring-opening reactions, resulting in the formation of different compounds or degradation products.

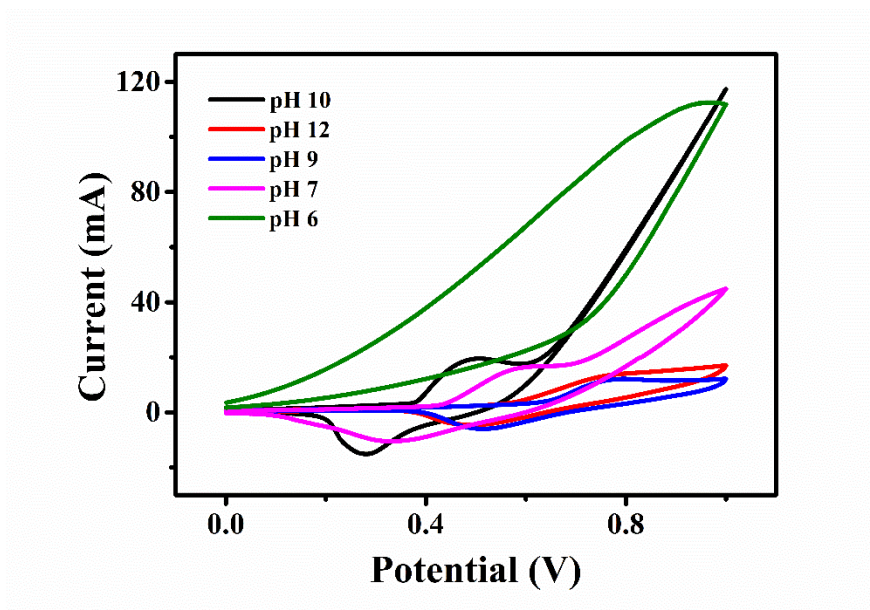


Figure S1: Effect of pH (from 6 to 10) of the NaOH electrolyte on the response of Ni-Fe LDO modified nickel foam sensor towards 0.01mM atrazine.

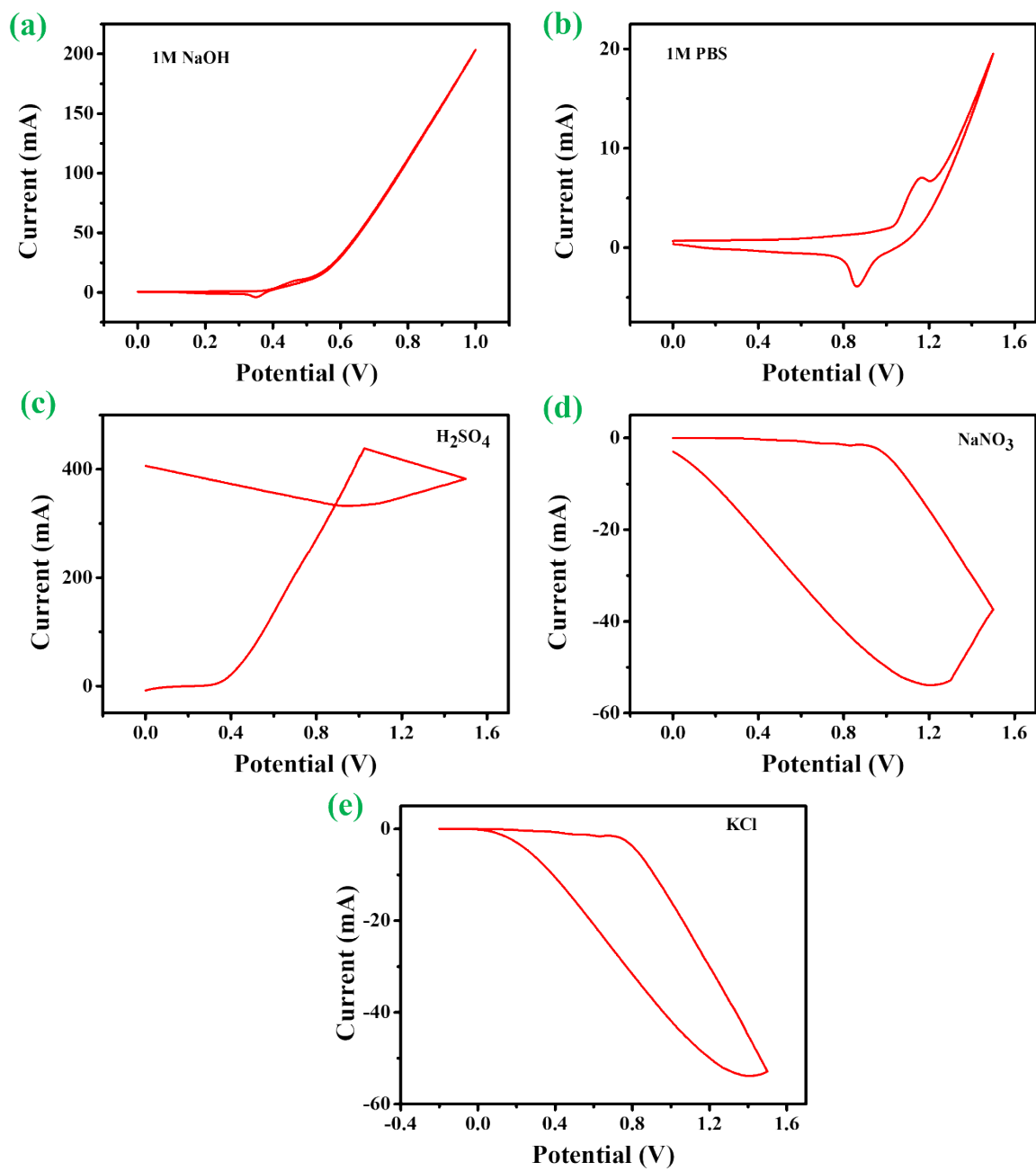


Figure S2: CV of LDO coated nickel foam electrode in the presence of atrazine in different electrolytes.

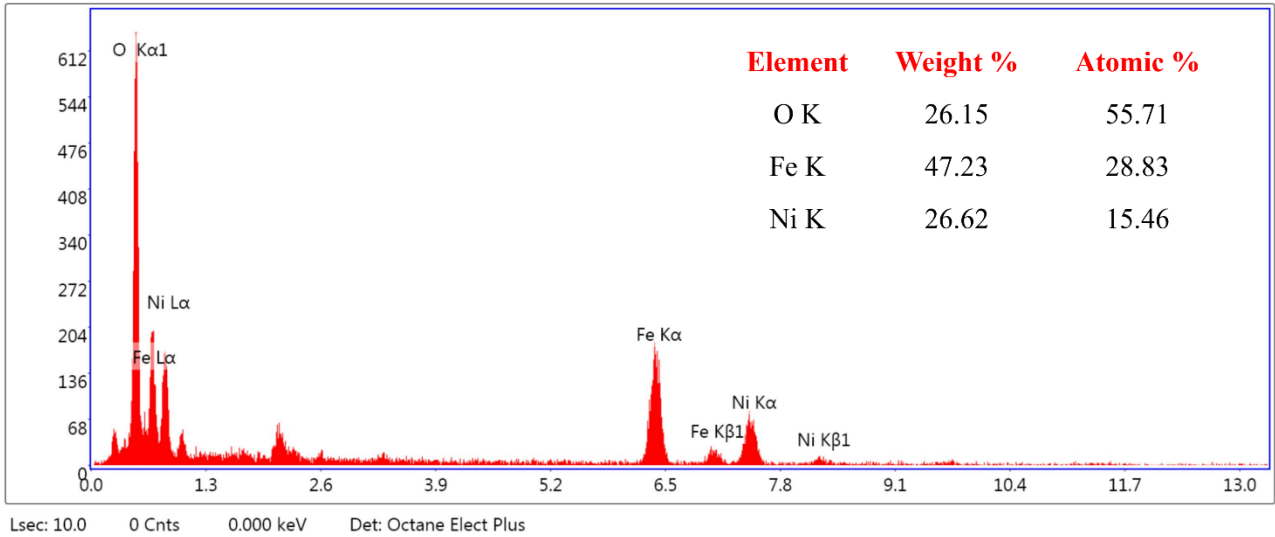


Figure s3: EDAX spectrum of Ni-Fe LDO

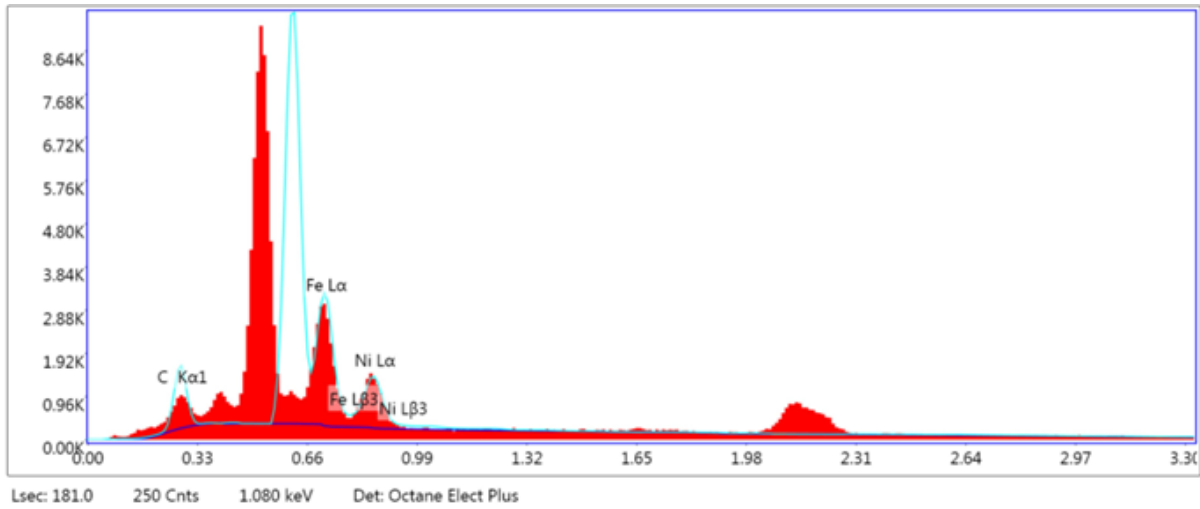


Figure s4: EDAX spectrum of Ni-Fe LDH

Element	Weight %	Atomic %
C	16.78	48.77
Fe	56.9	35.58
Ni	26.32	15.65

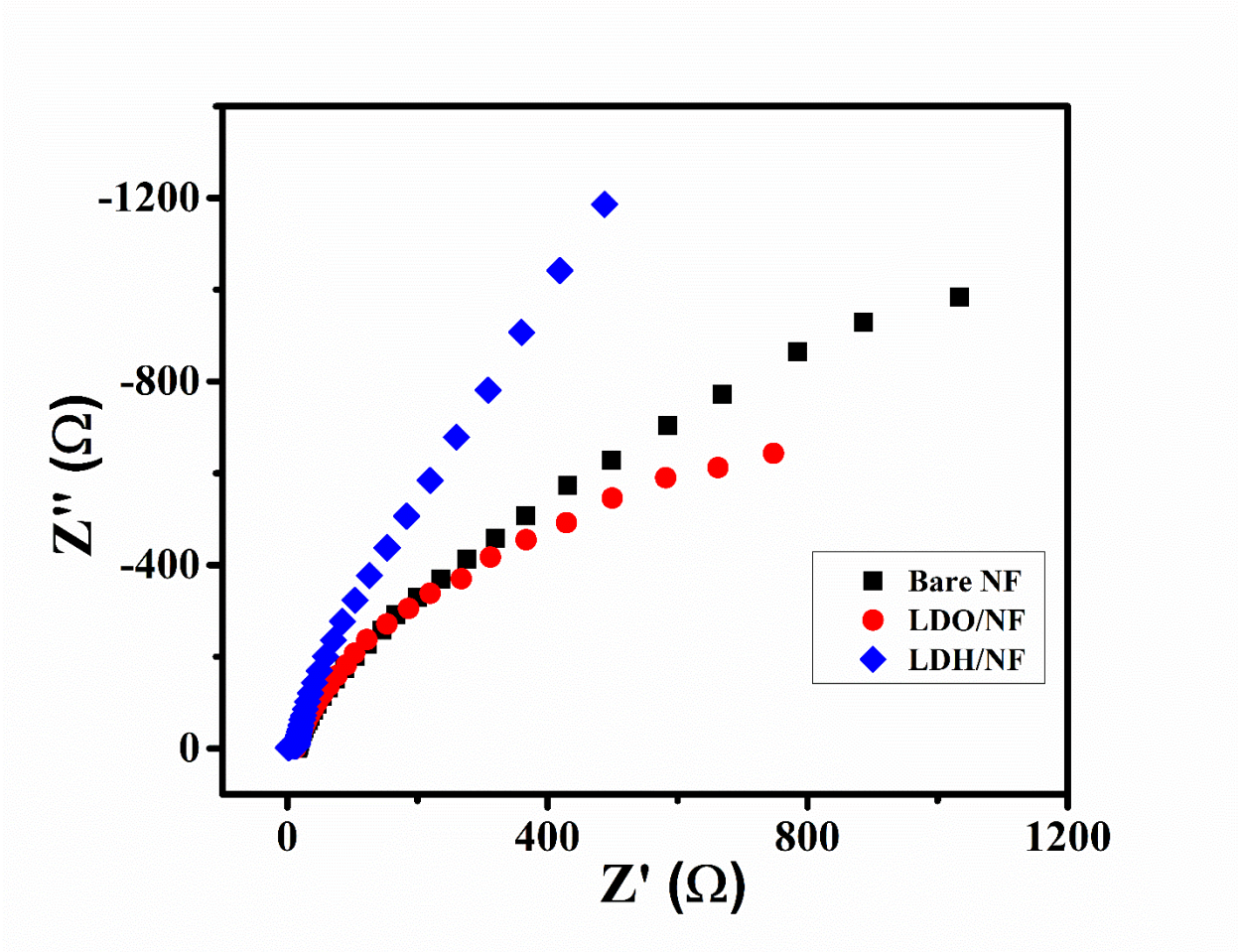


Figure s5: Nyquist plot of 3 different electrodes (1) bare NF and (2) LDH and LDO modified electrodes.

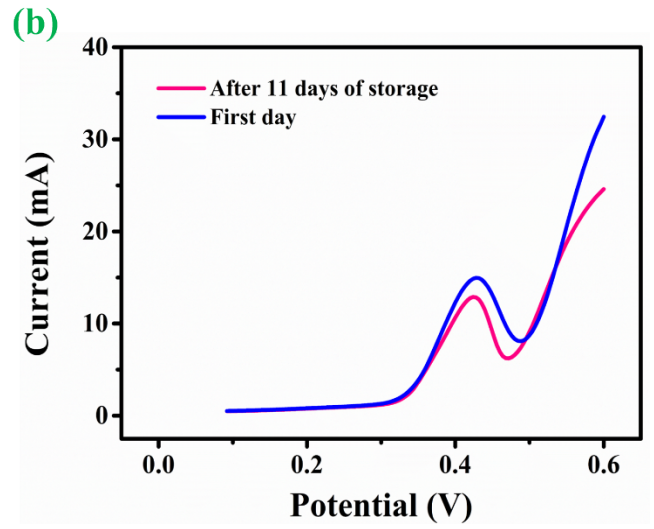
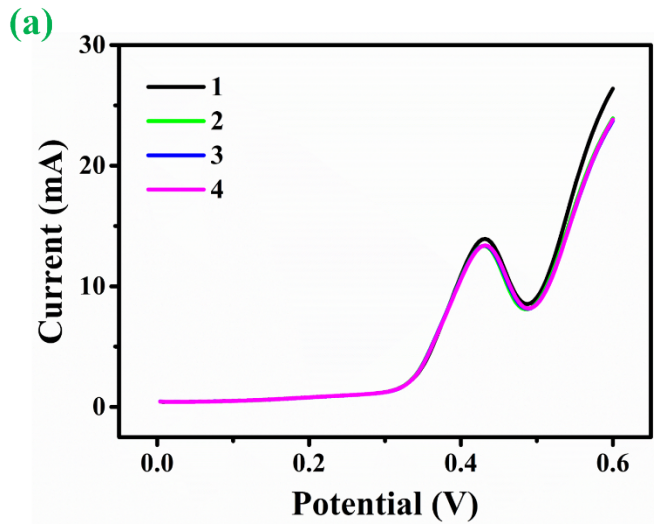


Figure s6: Repeatability and stability study