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Post synthetically modified Metal-Organic Framework as efficient Hydrogen evolution reaction catalyst in all *pH* conditions

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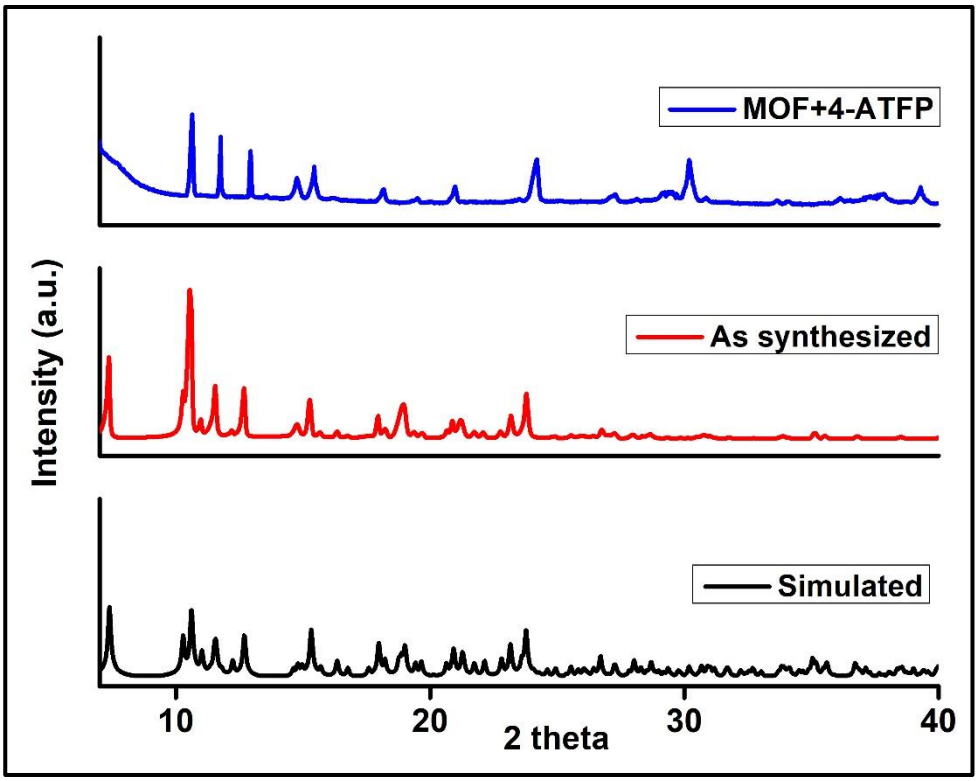
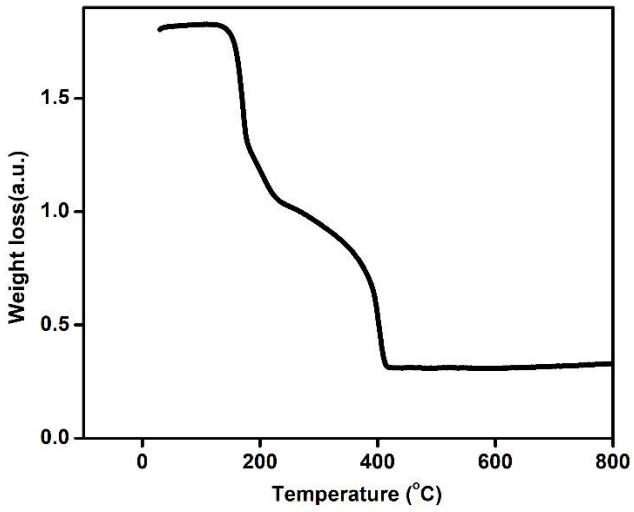
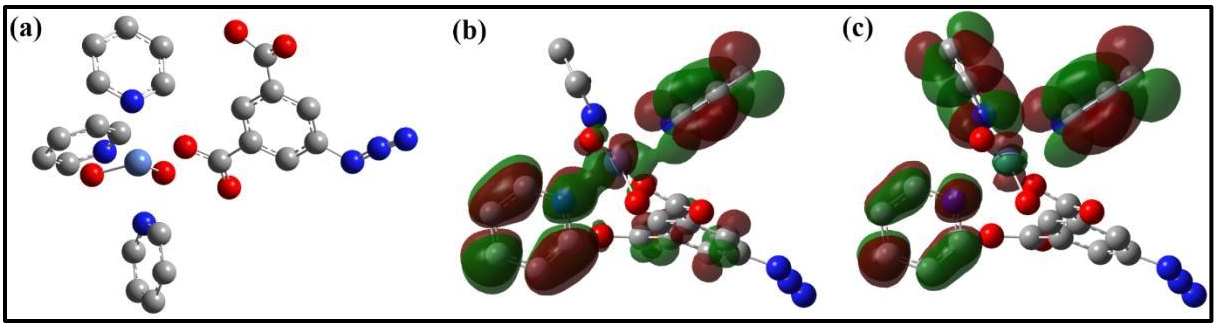


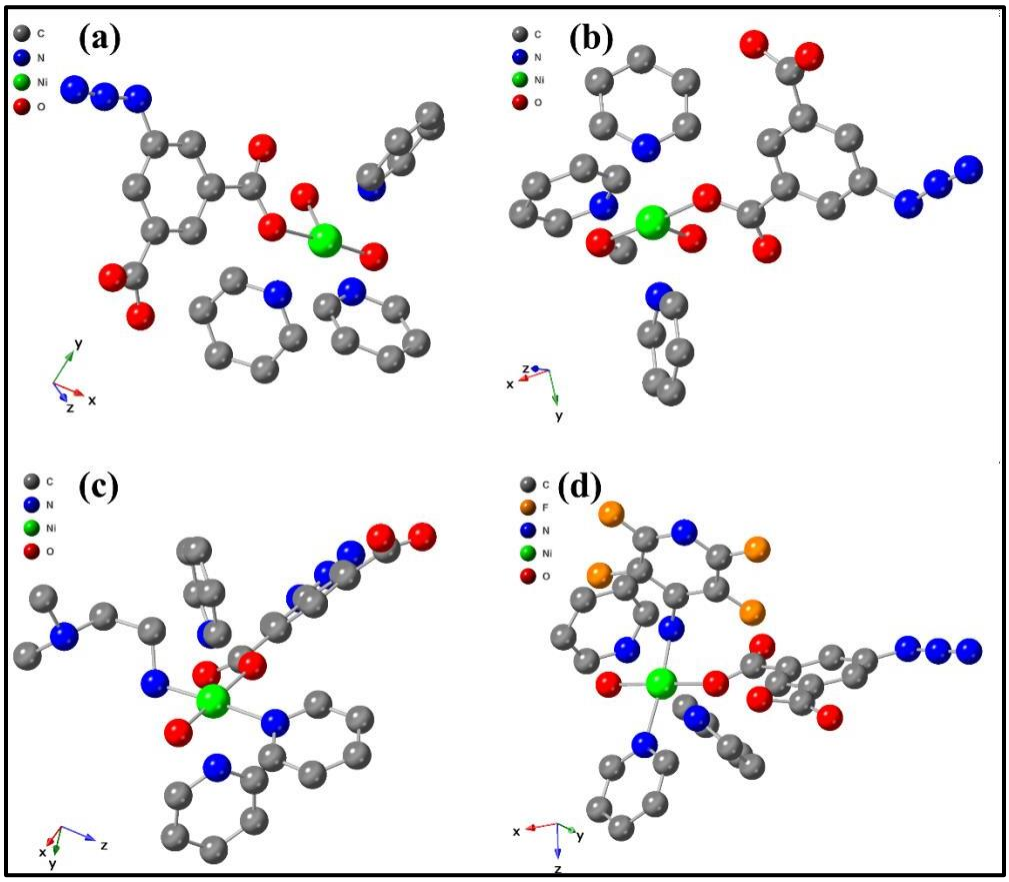
SI 1. XRD spectrums of simulated, as synthesized, and 4-ATFP substituted Niipa



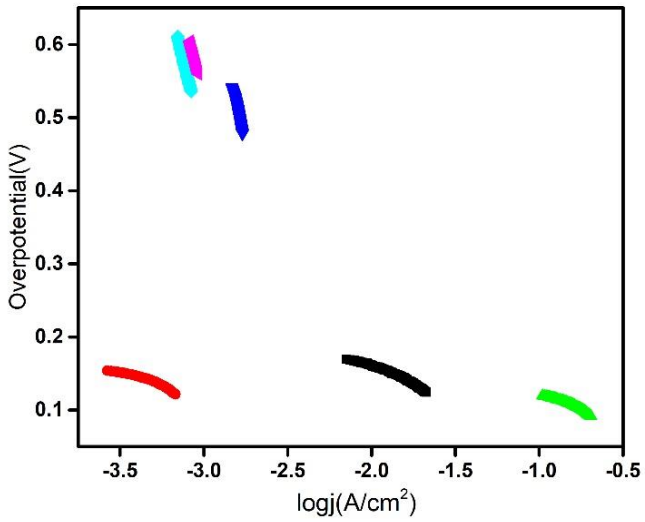
SI 2. TGA analysis of as synthesized Niipa



SI 3: (a) Optimized structure of Ni-MOF (1) precursor. C atoms are represented in black, N in blue, O in red, and Ni in cyan. (b) HOMO and (c) LUMO spin density plots for the ground state of (1). The transparent green and red orbital lobe colours designate excess α and β spins, respectively. The contour values are set to ±0.02 (e bohr -3)1/2. H atoms in all the pictures are omitted for clarity.



SI 4: Optimized structure of (a) Ni-MOF (1) precursor, and (b) methyl (1'), (c) N,N dimethyl ethylene diamine (2), (d) 4-amino tetrafluoro pyridine (3), substituted moieties. H atoms are omitted for clarity.



SI 5: Tafel slopes of bare MOF in neutral *pH* (cyan), acidic *pH* (purple), DMEDA substituted MOF in neutral *pH*(blue), and of 4-ATFP substituted MOF in acidic (green), alkaline (black) and neutral (red) solution

The Tafel slope of bare MOF in neutral condition is 866 mV, whereas that in acidic condition is 832 mV. For DMEDA substituted MOF in neutral condition, the Tafel slope is 659 mV.