Electronic Supplementary Information

Ionic Liquid *in-situ* Functionalized Carbon Nanotubes as Metal-Free Catalyst for Efficient Electrocatalytic Hydrogen Evolution Reaction

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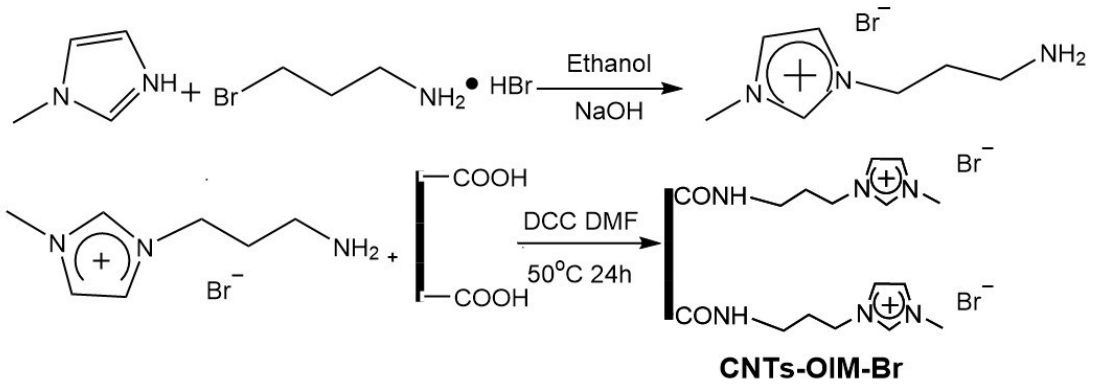

Scheme S1. Previous strategy of synthesizing CNTs-OIM-Br$^-$ electrocatalyst for comparison.

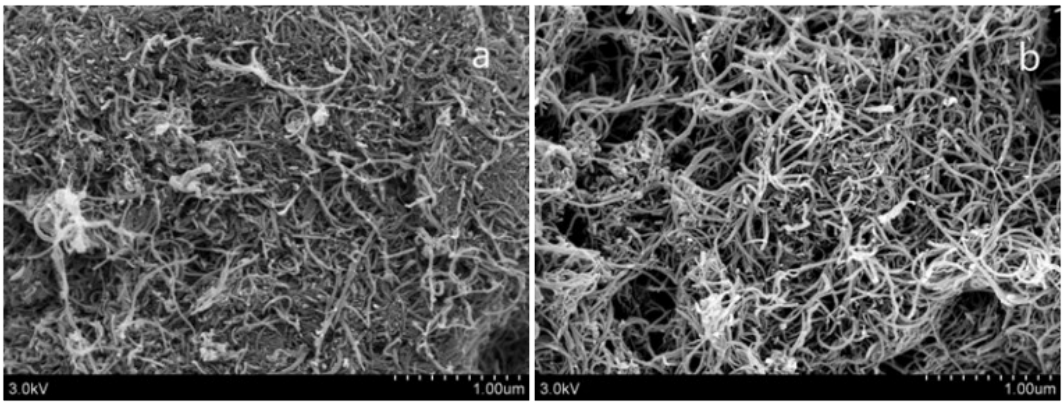

Fig. S1. SEM image of CNTs (a) and CNT-IM-Cl (b).

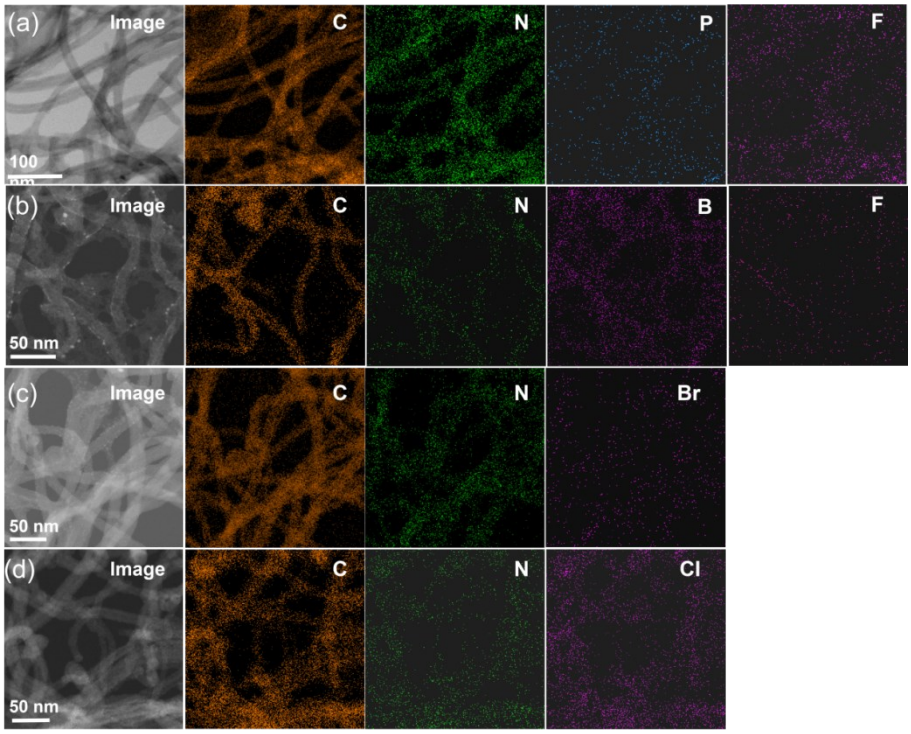

Fig. S2. TEM images and of CNT-IM-BF_4 (a), CNT-IM-PF_6 (b), CNT-IM-Br (c), and CNT-IM-Cl (d).

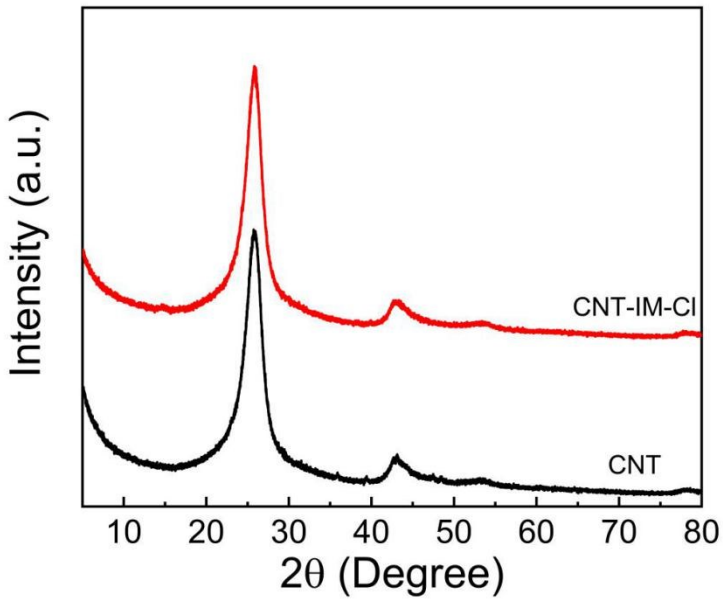

Fig. S3. XRD patterns of original CNT and imidazole functionalized CNT-IM-Cl.

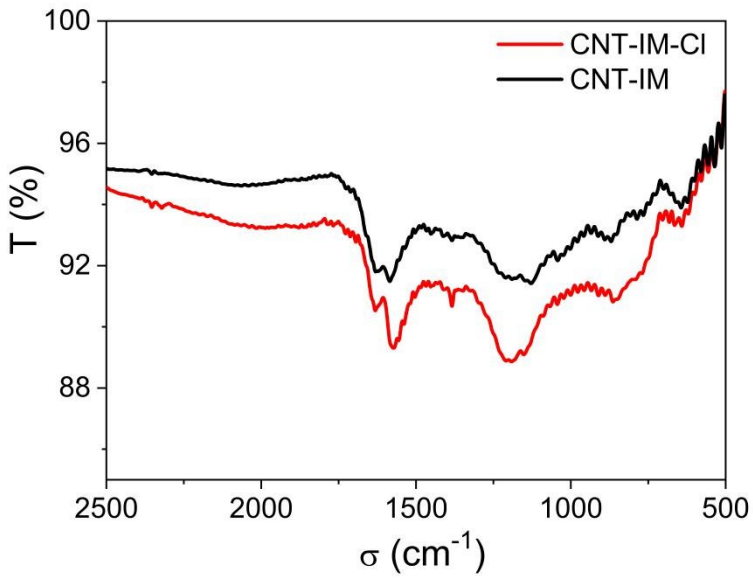

Fig. S4. FT-IR spectra of CNT-IM and CNT-IM-Cl.

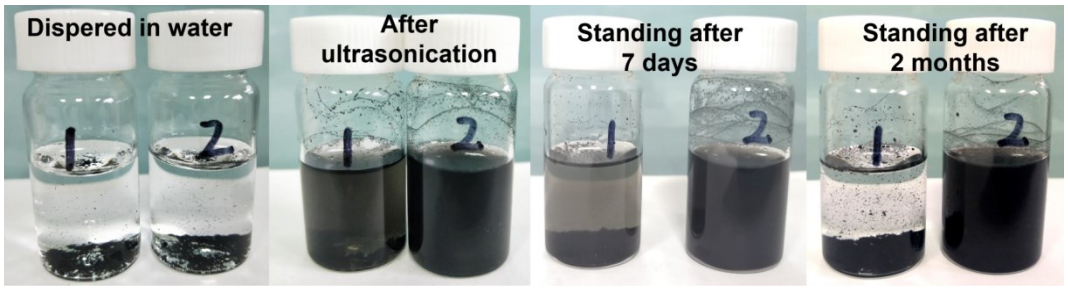

Fig. S5. Dispersity of CNT (1#) and CNT-IM-Cl (2#) in the water.

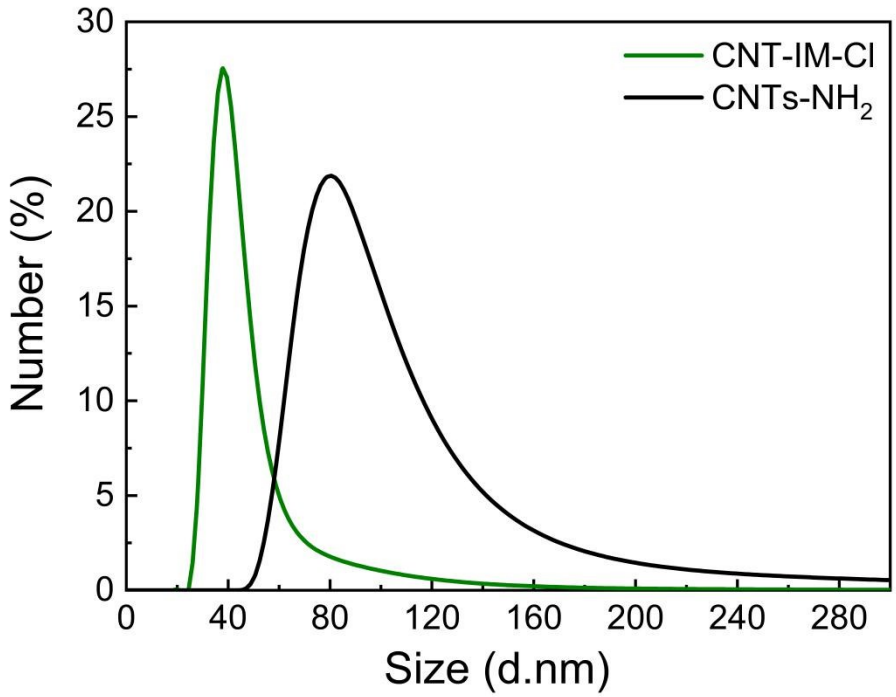

Fig. S6. Size distribution of CNT and CNT-IM-Cl.

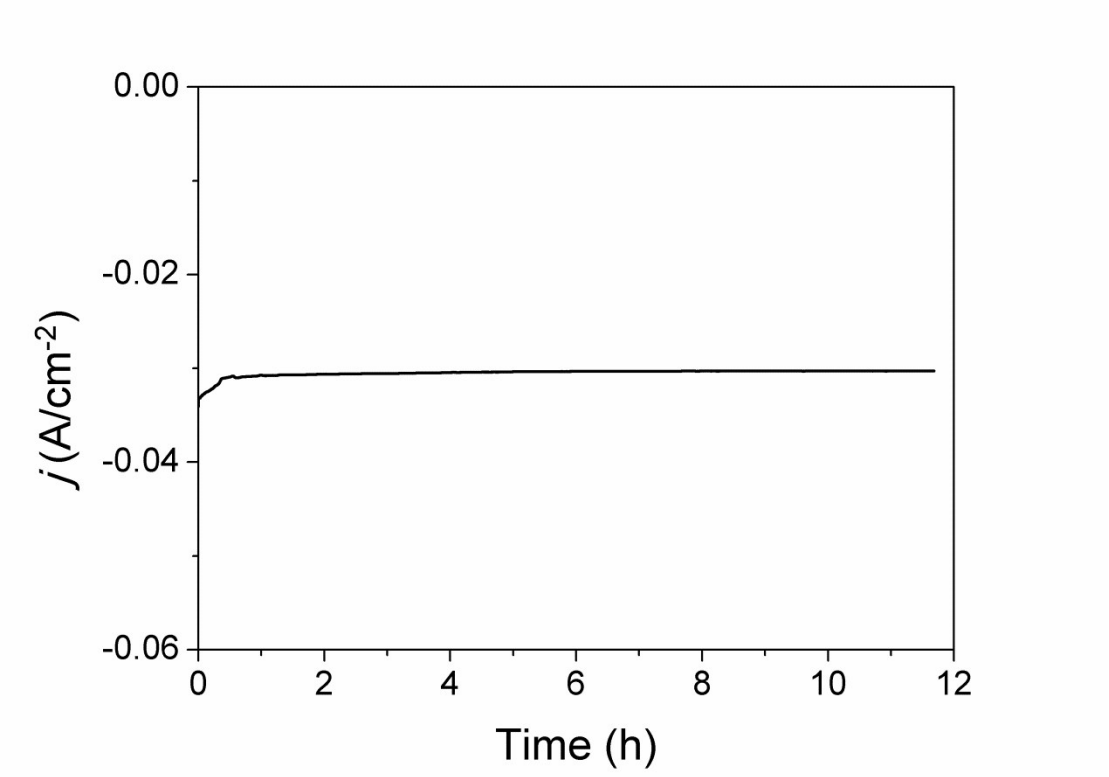

Fig. S7. Stability of CNT-IM-Cl catalyst during HER under current density of 35 mA cm^{-2}.

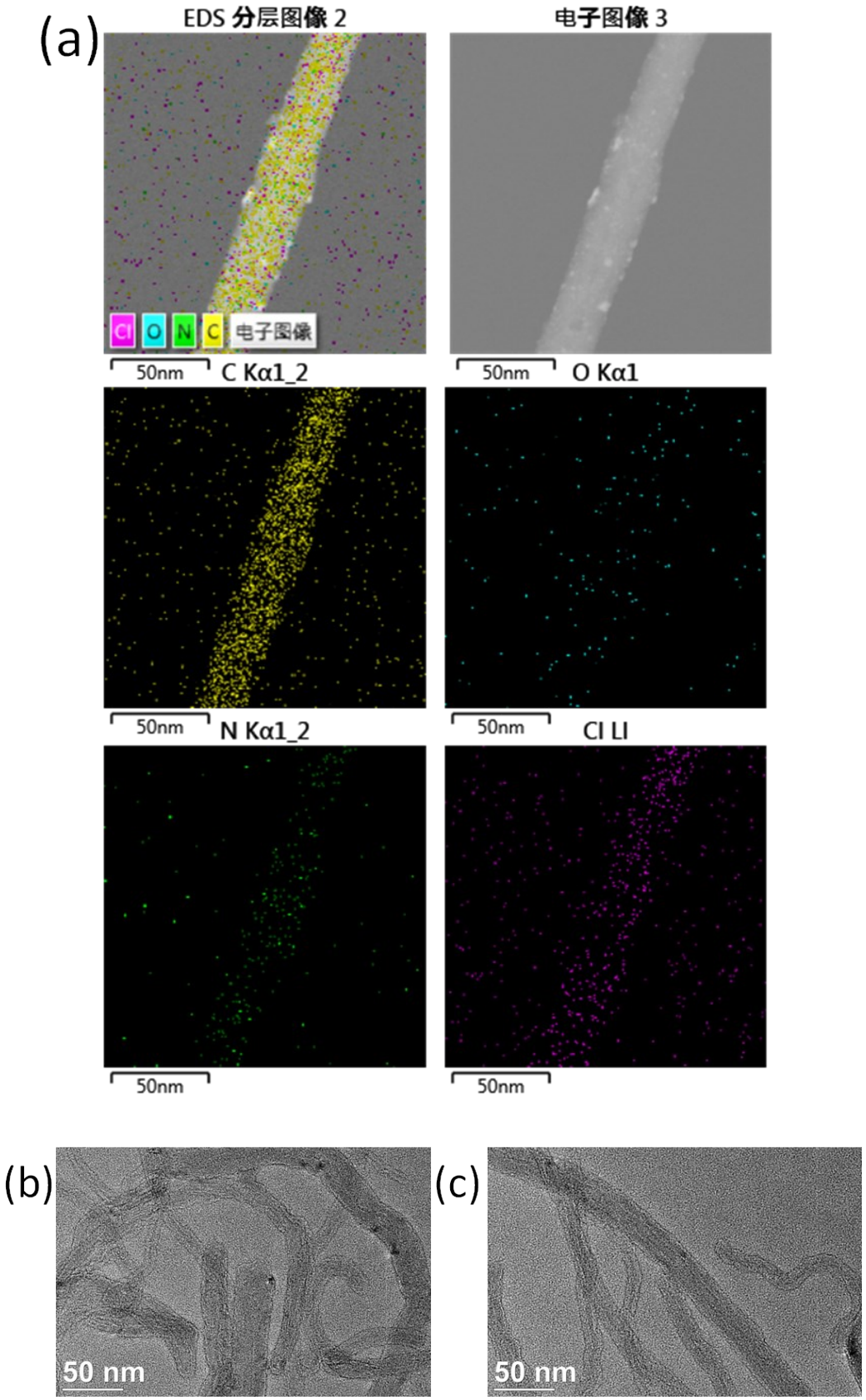

Fig. S8. (a) EDS mapping of CNT-IM-Cl after HER. (b) TEM image of CNT-IM-Cl before HER. (c) TEM image of CNT-IM-Cl after HER

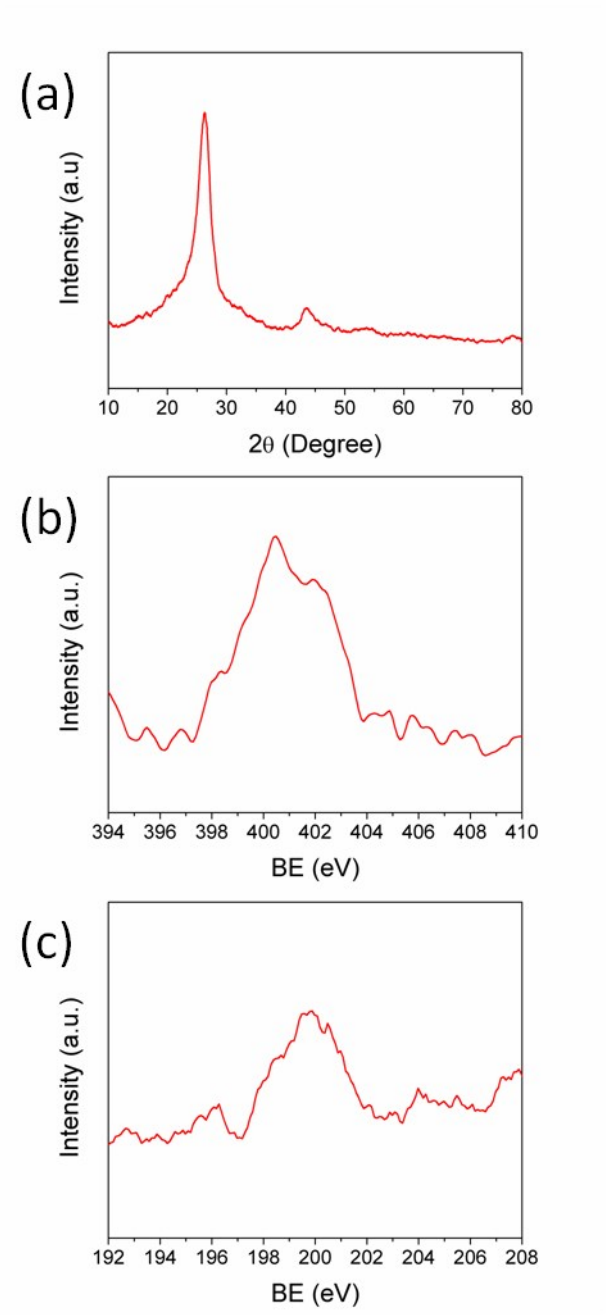

Fig. S9. (a) XRD pattern of CNT-IM-Cl after HER, N 1s spectrum (b) and Cl 2p spectra (c) of CNT-IM-Cl after HER.

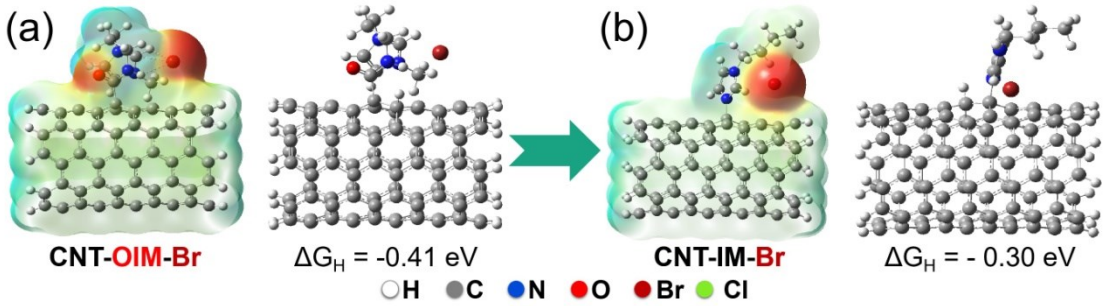

Figure S10. Theoretical study of surface electrostatic potential (blue: positive; red: negative; and green: neutral) and free energy of hydrogen adsorption on the CNT-OIM-Br (a) and CNT-IM-Br (b).

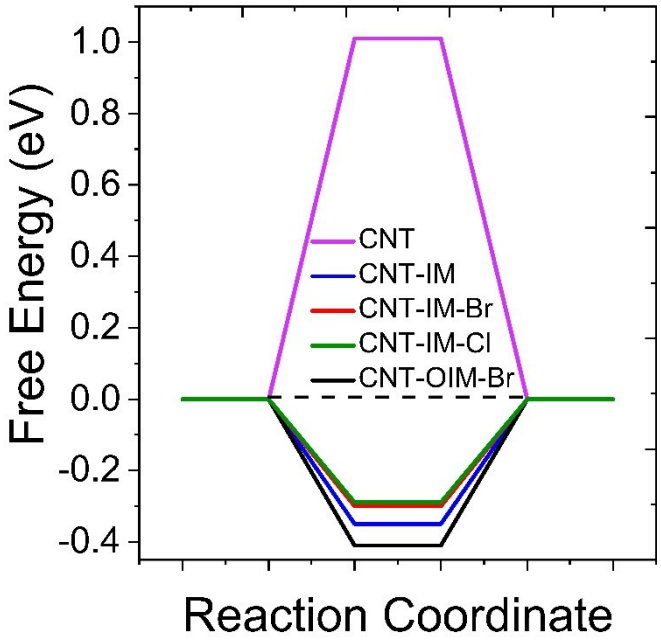

Fig. S11. Theoretical study of free energy of hydrogen adsorption on the CNT, CNT-IM, CNT-IM-Br, CNT-OIM-Br surface.

Table S1 Cl^- concentration in the electrolyte

	Cl^- concentration (mg/L)
Before HER	3.887
After HER	3.834

The Cl^- in the electrolyte (0.5 M H_2SO_4) is resulted from the impurity from H_2SO_4.