

Supporting Information

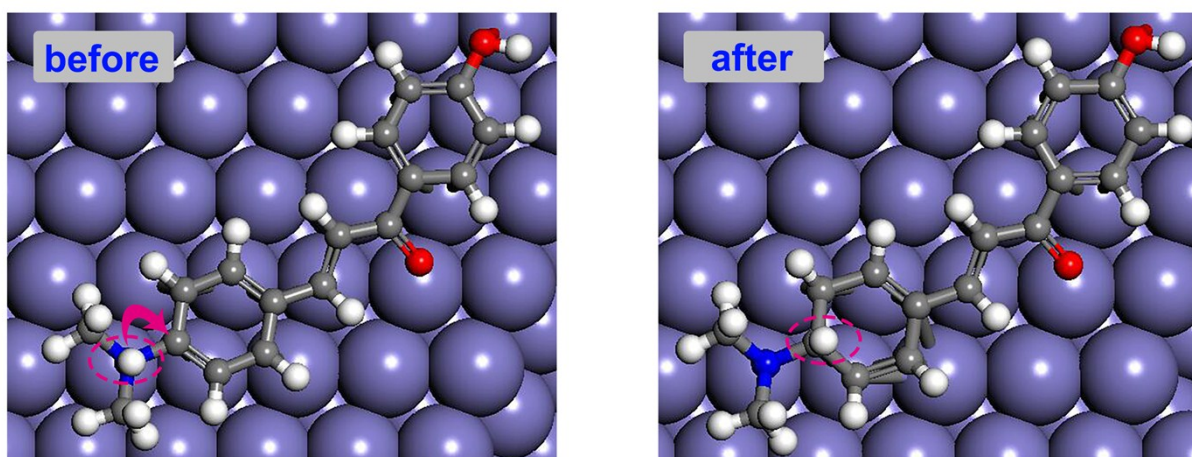


Fig. S1 Adsorption configurations of Inh3H before and after the geometry optimization.

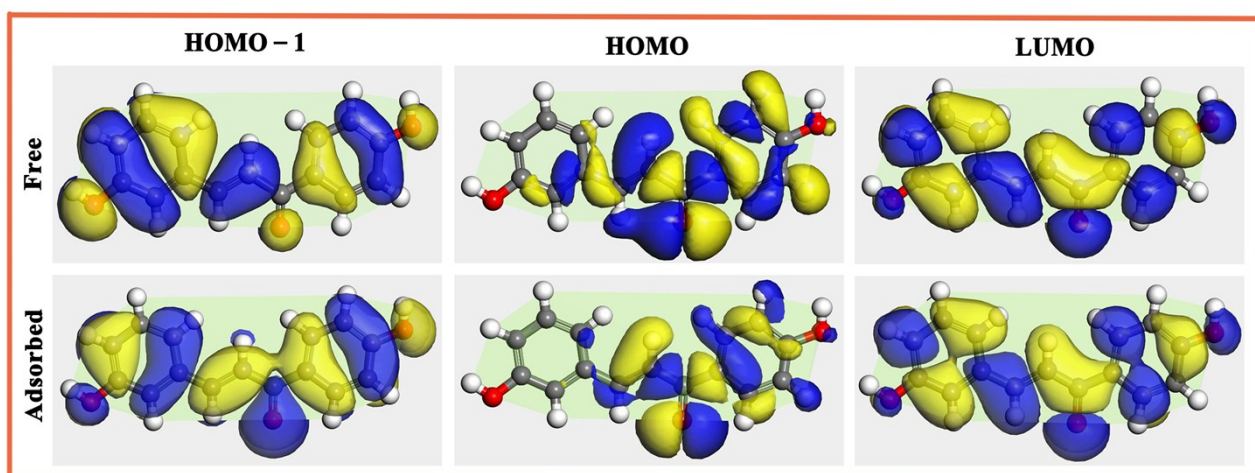


Fig. S2 Molecular orbital plots for the Inh2 molecule from the HOMO-1 to LUMO under the free (upper row) and adsorbed state (lower row).

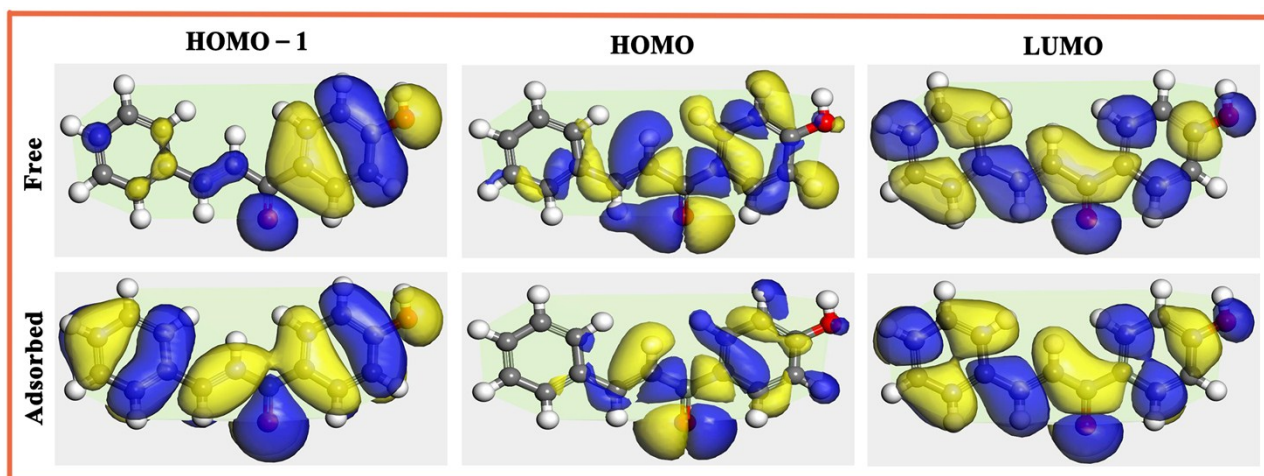


Fig. S3 Molecular orbital plots for the Inh1 molecule from the HOMO-1 to LUMO under the free (upper row) and adsorbed state (lower row).