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Aromatic heterocycle-grafted NH_2-MIL-125(Ti) via conjugated linker with enhanced photocatalytic activity for selective oxidation of alcohols under visible light

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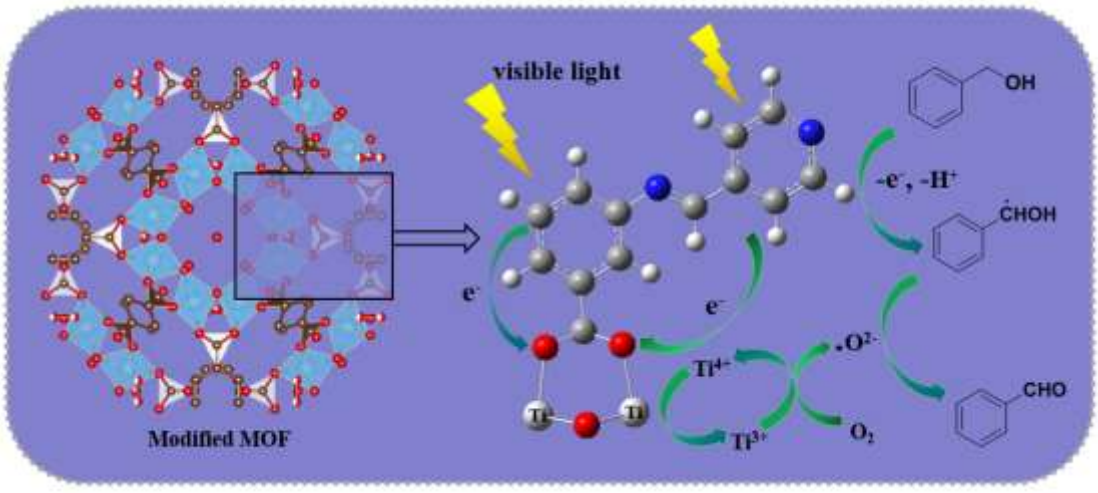
Graphical Abstract

alcohols under visible

light



A novel and facile post-grafting strategy, via a Schiff base chemical reaction between aldehyde and -NH_2 groups within NH_2-MIL-125(Ti) has been developed to construct aromatic heterocycle-grafted MOF photocatalysts. The improved conjugated system enhanced MOFs showed lower band gaps and their excellent catalytic activities were manifested by selective oxidation of alcohol to benzaldehyde under visible light irradiation with high conversion and selectivity. Density functional theory (DFT) was applied for simulating the band gaps and electron orbits of modified MOFs. The post-synthetic in the MOF network did not influence the