Ligand insertion in MOF-74 as effective design for oxidation of ethane to ethanol

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Efficient conversion of ethane into valuable materials is important with the availability of new natural gas resources. Recently, metal-organic frameworks (MOFs) with open iron sites (i.e. Fe$_{0.1}$Mg$_{1.9}$-MOF-74) have shown to be promising material for catalyzing ethane to ethanol reaction. In this computational study, various size-matching ligands are inserted to further optimize this reaction. Our density functional theory calculations show that the presence of ligands enhance the binding affinity of the oxygen atoms of N$_2$O to the iron centers in the framework, thereby leading to an improvement in the oxidizing process. Furthermore, the reaction pathway for the new structures show reduced enthalpy barrier in the rate-determining step in the oxidation of ethane reaction cycle. These findings provide blueprints in the performance of the Fe$_{0.1}$Mg$_{1.9}$-MOF-74 can be optimized for next-generation catalysts.