Computational design of ligand insertion in MOF-74 as catalyst for oxidation of ethane to ethanol

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Conversion of ethane into valuable materials attracts attention with the availability of new natural gas resources. Recently, metal-organic frameworks (MOFs) with open iron sites have shown to be promising candidates for catalyzing ethane to ethanol reaction. In this computational study, various different ligands are inserted to create newly designed Fe0.1Mg1.9-MOF-74. Density functional theory calculations indicate that the presence of ligands enhance the binding affinity of the oxygen atoms of N2O to the iron atoms in the framework, thereby leading to an improvement in the oxidizing process. Furthermore, compared with the new structure results in reduced enthalpy barrier in the rate-determining step in the oxidation of ethane reaction cycle. These findings provide ways in which one can optimize the performance of the Fe0.1Mg1.9-MOF-74 for next-generation catalysts.