9th European Chemistry Congress

June 17-18, 2019 | Berlin, Germany

Reaction mechanism and kinetic properties of IIIB transition metals Fe/Co/Ni and their metal oxides FeO/CoO/NiO for catalytic oxidation of methane to methanol: A reliable calculation strategy

Hongxia Liu
Anshan Normal University, China

The related energy and multi-channel oxidation of methane to methanol reaction potential energy surface under the IIIB transition metal and its oxide catalysts and its dynamic characterization have been investigated with the density functional calculations. The geometries were fully optimized by the B3LYP level. The calculation results show that the transition barriers and the reaction rate constant at 298 K all show oscillation modes, with the increase of atomic number. While the calculated reaction energies (Er/kcal mol^{-1}) and the energy of hyper conjugative interaction (E(2)) are gradually increased. The transition metal dioxide can be treated to form transition metal and oxygen, which can still be used as catalysts for methane oxidation and the generated oxygen can continuously be used as oxidants. We calculated the rate constant of this reaction pathway, the calculated dynamic characterization indicating that the rate constant has the positive temperature dependence. According, to the dynamic results and the energetically intermediates and transition states involved in the dominant paths, the reaction is expected to be occurred the most rapid under the catalysis of transition metal oxides. According to our calculation, the title reaction is exothermic reaction under the catalyst of transition metal oxides and it is a thermodynamically feasible reaction. The theoretical reference data on searching new catalysts to catalytic oxidation of methane will be offered.

Biography

Hongxia Liu has completed her PhD at Jilin University in China and Postdoctoral studies from University of Massachusetts. She is the Lecture of Inner Mongolia Normal University, a member of Inner Mongolia Key Laboratory of Green Catalysis. She has published more than 30 papers in reputed journals and has been serving as an Editorial Board Member of repute.

liuhx@imnu.edu.cn

Notes: