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Solventless C−C Coupling of Low Carbon Furanics to High Carbon Fuel Precursors Using an Improved Graphene Oxide Carbocatalyst

Authors : Ashish Bohre, Blaž Likozar, Saikat Dutta, Dionisios G. Vlachos, Basudeb Saha

Abstract : Graphene oxide, decorated with surface oxygen functionalities, has emerged as a sustainable alternative to precious metal catalysts for many reactions. Herein, we report for the first time that graphene oxide becomes super active for C-C coupling upon incorporation of multilayer crystalline features, highly oxidized surface, Brønsted acidic functionalities and defect sites on the surface and edges via modified oxidation. The resulting improved graphene oxide (IGO) demonstrates superior activity to commonly used framework zeolites for upgrading of low carbon biomass furanics to long carbon chain aviation fuel precursors. A maximum 95% yield of C15 fuel precursor with high selectivity is obtained at low temperature (60 C) and neat conditions via hydroxyalkylation/alkylation (HAA) of 2-methylfuran (2-MF) and furfural. The coupling of 2-MF with carbonyl molecules ranging from C3 to C6 produced the precursors of carbon numbers 12 to 21. The catalyst becomes inactive in the 4th cycle due to the loss of oxygen functionalities, defect sites and multilayer features; however, regains comparable activity upon regeneration. Extensive microscopic and spectroscopic characterization of the fresh and reused IGO is presented to elucidate high activity of IGO and to establish a correlation between activity and surface and structural properties. Kinetic Monte Carlo (KMC) and density functional theory (DFT) calculations are presented to further illustrate the surface features and the reaction mechanism.

Keywords : methacrylic acid, itaconic acid, biomass, monomer, solid base catalyst
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