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Catalytic Effects of Oxide Surfaces on Diels-Alder Cycloaddition between Furan and Methyl Acrylate: A DFT Study. TAHA SALAVATI-FARD, GLEN JENNESS, STAVROS CARATZOULAS, DOUGLAS DOREN, University of Delaware — Using density functional theory with periodic boundary conditions, we study the catalytic effects of oxide surfaces such as ZrO_2 and HfO_2 on Diels-Alder reaction between furan and methyl acrylate. The cycloadduct can be dehydrated later to produce methyl benzoic which is an important step toward benzoic acid production. The gas-phase and on-surface reaction mechanisms are studied in detail. The surface hydration effects on the reaction mechanism and energy profile are studied as well. Our calculations show that the oxide surfaces catalyze the reaction significantly through the interaction of metal sites with methyl acrylate. The calculations are interpreted by making use of electronic density of states and band structure of the catalyst.

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