

Abstract Submitted
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Catalysis in the Diels-Alder Cycloaddition of Biomass-Derived Furan and Methyl Acrylate by Transition Metal Oxide Surfaces.¹ TAHA SALAVATI-FARD, GLEN JENNESS, STAVROS CARATZOULAS, DOUGLAS DOREN, University of Delaware — Using computational methods, the catalytic effects of oxide surfaces on the Diels-Alder reaction between biomass-derived furan and methyl acrylate are investigated. The cycloadduct can be dehydrated later to produce methyl benzoic which is an important step toward benzoic acid production. Different systems such as clean, partially hydroxylated and fully hydroxylated ZrO₂ are considered. The Langmuir and Eley-Rideal mechanisms are studied, as well. Our calculations show that the oxide surfaces catalyze the reaction significantly through the interaction of metal sites with the electron-poor reactant. The calculations are interpreted by making use of the total and projected electronic density of states and band structure of the catalyst.

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