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Title: MgO/CaO Nanocomposite Facilitates Economical Production of d-Fructose and d-Allulose Using Glucose and Its Response Prediction Using a DNN Model Authors: Mahala, Sangeeta (/jspui/browse?type=author&value=Mahala%2C+Sangeeta) Devi, Bhawana (/jspui/browse?type=author&value=Devi%2C+Bhawana) Isomerization Keywords: Selectivity Magnesium oxide Issue Date: 2022 Publisher: **ACS Publications** Citation: Industrial and Engineering Chemistry Research, 61(6), 2524-2537 Abstract: This study presents a method for the economical production of fructose and allulose (a valuable byproduct) directly from glucose over a MgO/CaO nanocomposite under an aqueous condition. The catalyst containing MqO and CaO at equal proportions helped manipulate the inherent characteristics of CaO, particularly strong basicity and surface properties. The analytical characterizations revealed that the structural assembly is such that MgO settles at the surface to initiate the isomerization reaction by providing a higher number of weak/medium base sites. The CaO present beneath undertakes the sequential conversion of the enol-intermediate to ultimate fructose and byproducts (mannose and allulose). Thus, the catalyst accelerated the glucose interconversion to obtain a fructose yield as high as 33 wt % with 80% selectivity within 15 min. At the same time, it also initiated the C-3 fructose epimerization to yield allulose (a low-calorie sugar molecule). Moreover, the adopted deep neural network modeling well predicted the catalytic response with the MAE <5%. The technoeconomic analysis estimated the minimum selling price of different products to be US \$ ~4/kg (fructose), \$ ~4/kg (mannose), and \$ ~10/kg (allulose).

> https://doi.org/10.1021/acs.iecr.1c04631 (https://doi.org/10.1021/acs.iecr.1c04631) http://hdl.handle.net/123456789/4671 (http://hdl.handle.net/123456789/4671)

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