Catalyst screening for the conversion of Xylose to xylitol Using Density Functional Theory, DFT.

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Hydrogen is a clean and complete zero-emission fuel with high energy carrier efficiency, and with broad applications in modern energy technologies, like automobile fuel cells. Its cost is however high, and there is a need to generate this renewable energy from less expensive materials. The exploitation of biomass (e.g. Xylose) as an energy source to generate valuable chemicals such as Xylitol, which can ultimately be used as a starting material for hydrogen production is an intelligent technique for reducing the reliance of fossil fuels in today's society. Presently, there is no literature on the theoretical study for the hydrogenation of xylose to xylitol on catalyst surfaces and hence, the mechanisms behind the reaction is yet to be fully understood. In the present study, we investigated the mechanism for the hydrogenation of xylose on five monometallic surfaces including Ni (111), Pt (111), Rh (111), Pd (111) and Ru (0001) using theoretical DFT techniques. Here, the objectives are to explain and interpret the various occurrences not directly available in experiments and also to validate the reaction mechanisms.