

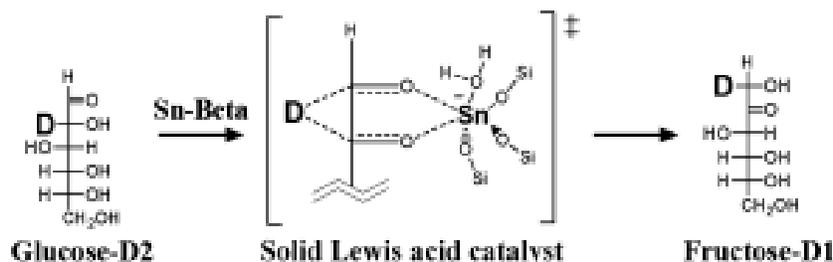


## Functionality of a Novel Biomass Conversion Catalyst Explained at the Atomistic Level

*This research was conducted by the group of Mark Davis at the California Institute of Technology.*

The core of catalytic chemistry research lies in understanding the role of a catalyst in a reaction. This understanding is crucial to the discovery of new materials leading to more energy efficient and benign chemical transformations. A critical reaction in utilization of the most abundant biomass ingredient, cellulose, is the conversion of glucose to fructose. Researchers at Caltech have now designed experiments to delineate the mechanism in this key chemical transformation catalyzed by a novel Sn-beta zeolite catalyst.

The research team replaced the hydrogen atom attached to the C-2 carbon of the glucose molecule with a deuterium atom and performed the experiments with and without the Sn-beta catalyst in pure water. Nuclear magnetic resonance (NMR) experiments demonstrate the ability of the catalyst to facilitate the intramolecular hydrogen transfer from C-2 to C-1 carbon atom of glucose. Furthermore, they provide testimony for (the first of its kind) Lewis acid catalysis in water. This finding is in stark contrast with the general belief that Lewis acidity is suppressed by the presence of water.<sup>[1]</sup> Given the fact that the Sn-beta catalyst is much more stable than the commercial enzymatic catalyst and active over a wide range of operating conditions, the findings of this work serve as a major milestone in developing catalysts for industrial scale biomass conversion process.



Isotopic labeling experiments reveal that an intra-hydride transfer rather than water mediated proton transfer converts abundant and inexpensive glucose to added-value fructose. In the transformation, the deuterium atom (D) shifts from the C-2 carbon atom in glucose to the C-1 carbon atom in fructose.

### RELEVANT PUBLICATION:

<sup>[1]</sup>Roman-Leshkov, Y.; Moliner, M.; Labinger, J.A.; Davis, M.E., “**Mechanism of glucose isomerization using a solid Lewis acid catalyst in water,**” *Angewandte Chemie-International Edition*, 4(47), 8954-8957 (2010). [DOI: 10.1002/anie.201004689]