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Exploring the mildest thermodynamic conditions for the inverse design of hydrogenation catalysts

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Designing green catalysts is the key for the development of next-generation technologies to convert biomass molecules into liquid fuels or other value-added chemicals. Recently, a few hydrogenation catalysts have been developed to effectively drive biomass conversions. However, designing hydrogenation catalysts that can work under mild conditions such as low pressure, low temperature, and green solvent remains a challenge. To provide the insights for designing greener hydrogenation catalysts, we explored the thermodynamics conditions (e.g., temperature, pressure, and solvents) for various hydrogenation or hydrogenolysis reaction based on biomass model compounds, by combining the Ab initio quantum chemistry calculations and experimental explorations. Our results show that thermodynamically it is indeed possible to design greener catalysts (e.g., robust and economic catalysts that work under mild conditions) for converting biomass molecules into value-added chemicals. In addition, we showed that optimal hydrogenation catalysts could be sought under the guidance of inverse design methods.

Biography

Dequan Xiao received a PhD degree in chemistry from Duke University. From 2009 to 2013, he worked as a Postdoctoral associate at Yale University. He is working as an Assistant Professor at the University of New Haven. His research interests focus on developing theoretical and computational chemistry methods to study materials properties and to perform inverse molecular design, for the applications in renewable energy science, soft matters, biophysics, and green chemistry. He has published 25 peer-reviewed articles, obtained 4 patents, and written two review articles on inverse molecular design and green catalysts for biomass conversion respectively.

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