Dequan Xiao, Organic Chem Curr Res 2014, 3:3
http://dx.doi.org/10.4172/2161-0401.S1.002

OMICS Group Conferences
Accelerating Scientific Discovery

International Summit on
Past and Present Research Systems of Green Chemistry
August 25-27, 2014 Hilton Philadelphia Airport, USA

Inverse molecular design of green catalysts for biomass conversion

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Owing to the development in modern theoretical and computational chemistry (e.g., density functional theory), predicting molecular properties using accurate and efficient quantum chemistry methods becomes more and more practical. As a consequence, inverse molecular design approaches based on quantum chemistry have emerged as an attractive computational approach to take on the challenges in materials discovery. In this presentation, the author will introduce an inverse molecular design method based on the tight-binding electronic structure theory and the scheme of linear-combination-of-atomic-potential (called TB-LCAP) for the design of green catalysts for biomass conversion. Approach of inverse molecular design aims at searching for optimum points on the hypersurfaces, defining the property-structure relationships, and then mapping out the molecular structures at the optimum points, leading to enhanced efficiency and success rate for material discovery. The author has applied the TB-LCAP inverse design method to successfully design nonlinear optical materials and dye-sensitized solar cells. In this talk, the author will present recent progress on developing the TB-LCAP method for the inverse design of green catalysts for biomass conversion.

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. Since 2013, 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 has written two review articles on *"Inverse molecular design" and "Green catalysts for biomass conversion"*.

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