ChE SEMINAR

Nano-Engineered Fischer-Tropsch Catalysts for Synfuel Production

Dr. Daniela Mainardi
Thomas C. & Nelda M. Jeffery Associate Professor and Chair of Chemical Engineering
Louisiana Tech University, Ruston, Louisiana, USA.
http://www2.latech.edu/~mainardi/

`

Seminar Room
Dept. of Chemical Engineering
Monday March 09, 2015: 4:00 PM

ABSTRACT

Due to the high dependence on fossil fuels, Fischer–Tropsch (FT) synthesis is attractive for the production of clean fuels. In general, FT synthesis transforms CO and H2 into long–chain liquid hydrocarbons. Despite extensive experimental and theoretical work conducted to date, several mechanistic details for FT synthesis remain unclear and unpredictable; specially the selectivity and reactivity of catalytic materials.

The work conducted by the Mainardi group employs multi-scale molecular simulation tools to nano-engineer FT catalysts. Using molecular simulations in combination with experiments lowers the costs related to design, as the simulations can be used to screen and suggest only the useful catalysts that can be subjected to experimental testing. In order to implement the FT process at a large scale, two fundamental issues need to be addressed, as they relate to the identification of the preferred sites for catalytic reactions to occur, the intermediate species in the FT process, and the preferred FT reaction pathway on a given catalyst surface.

The ultimate goal of this work is to provide insights into the design of novel nano-engineered FT catalysts that will alleviate energy and environmental issues in the medium and long term. Thus, in this work, promising core-shell binary nanocatalysts were design and investigated using electronic structure methods. Multi-scale molecular simulation tools were used to investigate the stability, activity, and

selectivity of core-shell FT catalysts as functions of the transition-metal type used..

ABOUT THE SPEAKER

Dr. Daniela Mainardi is an Associate Professor and the Program Chair of Chemical Engineering at Louisiana Tech University in the United States; currently holding the Thomas C. & Nelda M. Jeffery Professorship in Chemical Engineering.

Dr. Mainardi has extensive experience in a large variety of multi-scale molecular simulation tools and has conducted research on different and complementary nano- and bio-technology-related topics with applications to transport and catalysis. She has published 23 peer-reviewed articles, 51 conference papers, 6 book chapters, and has given 12 invited talks at international conferences, educational institutions, and research laboratories. Dr. Mainardi have participated in the organization of several international workshops, being her latest the “World Congress on Petrochemistry and Chemical Engineering”, that took place in November 2013 in San Antonio, Texas, USA. Dr. Mainardi has been nominated and selected Editorial Board Member of the Elsevier Editorial System for Surface Science, the Petrotex Publication Group, and the Chemical Sciences Journal. Dr. Mainardi has received the prestigious USA National Science Foundation (NSF)-CAREER award in 2005 for her work on Modified-Methanol Dehydrogenase Enzymatic Catalysts For Fuel Cell Devices.

Dr. Mainardi is a senior member of the USA American Institute of Chemical Engineers (AIChE) since 2010. She have been the Chair and Co-Chair for several AIChE Spring and National meetings, a Director (2009-2011) and Topical Chair (2010) of the AIChE-TEP Division, the 2010 Spring AIChE Meeting TEP Division Programming Chair, and an Advisory Board Member of the AIChE Center for Energy Initiatives. In 2012, Dr. Mainardi was publically nominated and elected Chair of the AIChE Transport and Energy Processes Division, and in 2013, she was honored to receive an AIChE Excellence and Service Award.