Contribution ID : **88** Type : **Invited Oral**

Rational Design of Nano-Catalysts for Sustainable Chemicals and Fuels: Insights from Theory and Simulation

Thursday, 16 August 2018 14:30 (45)

With the ever increasing consumption of the world's fossil-fuel resources due to the rapid development of industry, as well as climate change which is mainly induced by a surge in CO2 concentration in the atmosphere, both energy and environmental issues are two key problems facing humanity[1]. Over the last decade there has consequently been a substantial increase in innovative utilization of renewable and environmentally benign energy resources. In particular, with the globally increasing socio-political pressure to reduce CO2 emissions, CO2 has become a promising carbon source with a zero or even negative cost and practically unlimited availability for sustainable chemical manufacturing of hydrocarbon fuels and their derivatives. Central to further advancement in the creation of renewable and benign energy sources and environmental protection, is the breakthrough developments of new nanocatalysts.

In the present talk, an over-view and recent results based on first-principles theory calculations, in synergy with experiment will be presented for several key catalytic reactions. These include, the dry reforming of methane with carbon dioxide over a nickel based composite catalyst, conversion of methane and carbon dioxide to the higher value product chemical acetic acid over metal-exchanged zeolites[2], as well as ammonia synthesis from nitrogen reduction over graphitic carbon nitride[3]. Finally, results will be presented illustrating how theory and computation can aid in the screening of candidate materials for particular desired functionalities.

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3 H. Liu, P. Wu, H. Li, Z. Chen, X. Zeng, Y. Zhu, Y. Jiang, X. Liao, B. Haynes, J. Ye, C. Stampfl, J. Huang, submitted.

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Session Classification : Speaker Sessions and Seminars

Track Classification : Catalytic Materials and Processes