# Density Functional Theory for Heterogeneous Catalysis

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## Overview

Catalysis in general, and heterogeneous catalysis in particular, is critical to most industrial processes, including the manufacturing of fine, specialty, petro and agro chemicals, pharmaceuticals, cosmetics, foods, and polymers. Catalysis is also central to the generation of clean energy and to the protection of the environment. At present, catalysts are used in over 80% of all chemical industrial processes, and contribute directly or indirectly to ~35% of the world's GDP. Foundation of catalysis depends on chemical kinetics, which is a science for studying the reaction rates of chemical reactions, taking into account their reaction mechanism. Improved kinetic models could be developed when atomic processes on surfaces and the identification and characterization of surface species become available. In the present GIAN course, the status in the development of an understanding of surface chemistry will be discussed from a theoretical and computational perspective.

Density functional theory (DFT) has emerged as an attractive tool for computational study of chemical reactions. DFT calculations of heterogeneous reactions on catalyst surfaces can provide insights about the reactivity and mechanisms, and can potentially allow *in silico* screening and design of catalysts. In this course, a theoretical and practical introduction to computational techniques for studying chemical reaction kinetics will be presented. While the primary focus will be on DFT calculations, molecular dynamics (MD) technique will also be discussed as they allow for the explicit inclusion of thermal and coverage effects. The course will illustrate the application of these techniques to the study of surface-catalyzed reactions by considering the steam reforming of alcohols (to generate hydrogen) on catalyst surfaces as a representative case. The participants will be introduced to the calculation of adsorption energies of molecules on surfaces, identification of transition states, reaction pathways and estimation of reaction rates. The open-source quantum chemistry software CP2K will be used for demonstrating all the computational methods as well as for the hands-on tutorial sessions.

| **Modules** | **Density Functional Theory for Heterogeneous Catalysis** |
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| **You Should Attend If…** | • You are a PG/UG student studying physics, chemistry, materials science, mechanical, chemical, bio-chemical engineering and interested to know and learn about chemical catalysis and kinetics modelling through density functional theory (DFT) with advanced molecular dynamics (MD) techniques<br>• You are an executive/engineer of an industry who is interested in chemical kinetic modelling through quantum chemical and molecular simulation techniques<br>• You are a scientist in an R&D laboratory and use/want to explore the chemical kinetic modelling through DFT and MD techniques<br>• You are a research scholar or faculty in an academic institution and want to explore the chemical kinetic modelling through DFT and MD techniques |
| **Fees** | The participation fees for taking the course is as follows:<br>**Participants from abroad : US $500**<br>**Industry/ Research Organizations: Rs. 15000**<br>**Academic Institutions:**<br>**Student: Rs. 1000 (Refundable subject to joining the course)**<br>**Faculty: Rs. 5000**<br>The above fee includes all instructional materials, computer use for tutorials and assignments, 24 hr free internet facility. The participants will be provided with accommodation on payment basis. |

# The Faculty

**Dr. Neeraj Rai** is an Assistant Professor in the Dave C. Swalm School of Chemical Engineering, Mississippi State University. His research interests include statistical mechanics, computational chemistry, catalysis, hierarchical systems, and optoelectronic materials

**Dr. Amit Kumar** is an Associate Professor in the Department of Chemical Engineering, Indian Institute of Technology Guwahati. His research interests include molecular modeling and simulation of porous materials, polymers, nanocomposites, gas adsorption and diffusion.

**Dr. Rajesh Kumar Upadhyay** is an Associate Professor in the Department of Chemical Engineering, Indian Institute of Technology Guwahati. His research interests include catalysis, membrane reactor, multiphase flow and flow measurement techniques.

## Course Dates:

06–11 August, 2018

## Course Coordinators

**Dr. Amit Kumar**
Phone: 0361 2582274
E-mail: amitkumar@iitg.ac.in

**Dr. Rajesh K. Upadhyay**
Phone: 0361 2582275
E-mail: rkupadhyay@iitg.ac.in

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Website URL: http://www.gian.iitkgp.ac.in/GREGN/index