



# ANAND MOHAN VERMA

Post-Doctoral Fellow

Chemical Engineering

Indian Institute of Science, Bangalore



## SHORT BIO

I hail from a beautiful town called Pepeganj, which is situated in Gorakhpur, Uttar Pradesh, India. I earned my BE and PhD degrees in Chemical Engineering from SLIET and IIT Guwahati, respectively. I am currently serving as a Research Associate - III in the Department of Chemical Engineering at the IISc, Bengaluru, India. Previously, I have worked as a Postdoctoral Researcher (Supervisor: Prof. Karoliina Honkala) and as a Visiting Research Fellow (Supervisor: Prof. Andreas Heyden) at the University of Jyväskylä (Finland) and the University of South Carolina (USA), respectively.

My current research interests lie in the areas such as bio-oil/biofuels upgrading, 2D materials, water splitting, fluxional catalysts, electrocatalytic CO<sub>2</sub> reduction and polyol oxidation, and others. For these research problems, I carry out extensive computer simulations on HPC machines using computational chemistry software packages such as GPAW, VASP, Gaussian, and Materials Studio.

## CURRENT RESEARCH

At the IISc Bengaluru, I am working on the projects such as machine learning assisted thermocatalytic CO<sub>2</sub> reduction reaction on (bifunctional) copper surfaces, water splitting and nitrogen reduction reactions on advanced 2D materials, and others using computational heterogeneous and electrocatalysis.

## CONTACT

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## EDUCATION

**PhD, Chemical Engineering**  
**Indian Institute of Technology, Guwahati**

2014 - 2018

Thesis title: Density Functional Theory Investigations on Upgrading of Phenolic Catalogue of Unprocessed Bio-Oil

Thesis Advisor: Prof. Nanda Kishore

**BE, Chemical Engineering**  
**Sant Longowal Institute of Engineering and Technology (SLIET), Punjab**

2010 - 2013

**Diploma, Chemical Engineering**  
**Government Polytechnic Gorakhpur, U. P.**

2007 - 2010

## WORK EXPERIENCE AND FELLOWSHIPS

**University of Jyväskylä (Finland), Post-Doctoral Fellow**

April 2019–December 2020

**MMMUT, Gorakhpur (India), Post-Doctoral Fellow**

February 2019–March 2019

**University of South Carolina (USA), Visiting Research Fellow**

January 2018–June 2018

## SELECTED PUBLICATIONS

A M Verma, M M Melander, and K Honkala, "On the mechanistic origins of the pH-dependency in Au-catalyzed glycerol electro-oxidation: insight from first principles calculations", *ACS Catalysis*, in press (accepted), 2021

A M Verma, K Honkala, and M M Melander, "Computational Screening of Doped Graphene Electrodes for Alkaline CO<sub>2</sub> Reduction", *Frontiers in Energy Research*, 8, 388(1-15), 2021.

M M Kauppinen, V Korpelin, A M Verma, M M Melander, and K Honkala, "Escaping scaling relationships for water dissociation at interfacial sites of zirconia-supported Rh and Pt clusters", *Journal of Chemical Physics*, 151, 164302(1-11), 2019

A M Verma and N Kishore, "Molecular Modeling Approach to Elucidate Gas Phase Hydrodeoxygenation of Guaiacol over a Pd(111) Catalyst within DFT Framework", *Journal of Molecular Modelling*, 24, 254(1-16), 2018

A M Verma and N Kishore, "Molecular Simulations of Palladium Catalysed Hydrodeoxygenation of 2-Hydroxybenzaldehyde using Density Functional Theory", *Physical Chemistry Chemical Physics*, 19, 25582-25597, 2017