# CURRICULUM VITAE

**ANAND MOHAN VERMA, PhD**

***Correspondence Address:***
Department of Chemical Engineering,
MNNIT Allahabad, India - 211004
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## Current Position

**Assistant Professor** in the Department of Chemical Engineering at the Motilal Nehru National Institute of Technology (MNNIT) Allahabad, Prayagraj, India – 211004 (Aug 2023 – till date).

## Research Interests

**General:** Density functional theory, computational heterogeneous- and electro-catalysis, reaction mechanisms, microkinetic modelling, and machine learning

**Specific:** Thermocatalytic/electrocatalytic $CO_2$ reduction, Bio-oils/Biofuels upgrading, polyol oxidation, advanced 2D materials, and water splitting

## Selected Publications*

*full list is given afterwards

1. **Anand M. Verma**, Laura Laverdure, Marko M. Melander, and Karoliina Honkala, "Mechanistic Origins of the pH Dependency in Au-Catalyzed Glycerol Electro-oxidation: Insight from First-Principles Calculations", ***ACS Catalysis***, 12, 662-675, 2022.
2. **Anand M. Verma**, Karoliina Honkala, and Marko M. Melander, "Computational Screening of Doped Graphene Electrodes for Alkaline $CO_2$ Reduction", ***Frontiers in Energy Research***, 8, 606742 (1-15), 2021.
3. **Anand M. Verma** and Nanda Kishore, "First-Principles Study on Gas-Phase Decomposition of Bio-oil Oxygenated Compounds over Palladium Catalyst Surface", ***Physical Chemistry Chemical Physics***, 21, 22320-22330, 2019.
4. Mohammad Saleheen, **Anand M. Verma**, Osman Mamun, Jianmin Lu, and Andreas Heyden, "Investigation of Solvent Effects on the Hydrodeoxygenation of Guaiacol over Ru Catalysts", ***Catalysis Science & Technology***, 9, 6253-6273, 2019.
5. **Anand M. Verma** and Nanda Kishore, "Molecular Simulations of Palladium Catalysed Hydrodeoxygenation of 2-Hydroxybenzaldehyde using Density Functional Theory", ***Physical Chemistry Chemical Physics,*** 19, 25582-25597, 2017.

## Academic Qualifications

- **Doctor of Philosophy (PhD)** (Specialization: ***Chemical Engineering***) (Course work CGPA: **7.67**)
  - Indian Institute of Technology (IIT) Guwahati, India (Jan 2014 – Jul 2018)

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

➢ **Bachelor of Engineering (BE)** (Specialization: ***Chemical Engineering***) (CGPA: **8.55**)

- Sant Longowal Institute of Engineering and Technology (SLIET), India (Aug 2010 – Jul 2013)
- **Thesis Title**: Characterization of Biodiesel Produced from Waste Soybean Oil

➢ **Diploma in Engineering** (Specialization: ***Chemical Engineering***) (Percentage: **77.48 %**)

- Government Polytechnic Gorakhpur, U. P., India (Jul 2007 – Jun 2010)
- **Project Title**: Design of Shell and Tube Heat Exchanger

➢ **10th (High School)** (Specialization: ***Maths and Science***) (Percentage: **61.83 %**)

- Bapu Inter College, U. P. Board, Allahabad, India (Jul 2006 – Jun 2007)

## Academic/Industrial Experiences

➢ **(CV Raman) Postdoctoral Fellow** at the **Indian Institute of Science**, Bengaluru, India (Mar 2021 – Aug 2023) (Supervisor: **Prof. Ananth Govind Rajan**)

- **Project Title:** *Using Density Functional Theory and Machine Learning to predict Catalysts for Thermochemical $CO_2$ Conversion to 1-Butanol*

➢ **Postdoctoral Research Associate** at the **University of Jyväskylä**, Finland (Apr 2019 – Dec 2020) (Supervisor: **Prof. Karoliina Honkala**)

- **Project Title:** *Heterogeneous and Electrocatalytic Oxidation of Biomass-derived Polyols at the Liquid-Solid Interface*

➢ **Postdoctoral Research Associate** at the **Madan Mohan Malviya University of Technology (MMMUT)**, Gorakhpur, India (Feb 2019 – Mar 2019) (Supervisor: **Dr. Satya Pal Singh**)

- **Project Title:** *Atmospheric Oxidation of Biogenic Volatile Organic Compounds using First Principles Methods*

➢ **Visiting Research Fellow** at the **University of South Carolina (UofSC)**, USA (Jan 2018 – Jun 2018) (Supervisor: **Prof. Andreas Heyden**)

- **Project Title:** *Elucidation of Hydrogenation Mechanism of Phenol over Various Noble Metal Surfaces*

➢ **Research Scholar** at the **Indian Institute of Technology (IIT) Guwahati**, India (Jan 2014 – Jul 2018)

- **Project Title:** *Density Functional Theory Investigations on Upgrading of Phenolic Catalogue of Unprocessed Bio-Oil*

➢ **Vocational Trainee** at the **National Fertilizers Limited**, Nangal, India, (Jun 2013 – July 2013)

- **Project Title:** *Industrial Productions of Ammonia, Urea, and Phosphoric Acid*

➢ **Vocational Trainee** at **Asian Fertilizers Limited**, Gorakhpur, India (May 2009 – Jun 2009)

- **Project Title:** *Understanding the Productions of Sulfuric Acid and Single Superphosphate*

## Computer Skills

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|---|---|---|
| **DFT Packages** | **:** | GPAW, ASE, Gaussian, VASP, Material Studio |
| **Operating Systems** | **:** | Linux (Ubuntu, Fedora, Red Hat), Windows |
| **Utility Software** | **:** | MS Office, LaTeX (Overleaf), Mendeley, Oracle VM |

**Super-Computers** : Cori, Comet, Stampede2, Mahti, Puhti, Param Pravega/Ishan
**Coding** : Python (basic), BASH (intermediate), C++ (basic)

## Course Works

- Introduction to Machine Learning, Dr. Clint P George
- Advanced Transport Phenomena (**CL 501**), Dr. A. Lakshmi & Dr. A. K. Ghoshal
- Computational Fluid Dynamics (chemical engineering aspects) (**CL 613**), Dr. A. Singh
- Computational Fluid Dynamics (mechanical engineering aspects) (**ME 543**), Dr. A. Dalal
- Optimization Techniques (**CL 615**), Dr. S. S. Murugan & Dr. R. Uppaluri
- Fluidization Techniques (**CL 614**), Dr. Subrata Kr. Majumdar
- Viscous Flow (**ME 648**), Dr. A. Dalal

## Teaching Assistances

- Molecular Simulations, (**CL 622**), Dr. Ashok Kr. DasMahapatra
- Multiphase Flow, (**CL 627**), Dr. Rajesh Kr. Upadhyay
- Engineering Drawing, (**ME 111**), Dr. Rajesh Kr. Upadhyay
- Chemical Engineering Thermodynamics, (**CL 207**), Dr. Partho Sarathi
- Advanced Transport Phenomena, (**CL 501**), Dr. N. Kishore
- Thermodynamic Lab, (**CL 211**), Dr. N. Kishore & Dr. K. Mohanti

## Professional Recognitions/Achievements

- **CV Raman Postdoctoral Fellowship** at the **Indian Institute of Science, Bengaluru (India)** under the supervision of Prof. Ananth Govind Rajan (Jan 2023)
- **Postdoctoral Fellowship** at the **University of Jyväskylä (Finland)** under the supervision of Prof. Karoliina Honkala (Apr 2019 – Dec 2020)
- **Visiting Research Fellowship** at the **University of South Carolina (USA)** under the supervision of Prof. Andreas Heyden (Jan 2018 – Jun 2018)
- **Travel Grant** by the **Ghent University**, **Belgium** (2018)
- Secured **1$^{st}$ position** in **Paper Presentation** event of **REFLUX-2018** for "Gas Phase Kinetic Investigations of Decomposition of Salicylaldehyde over Pd(111) Catalyst Surface" (2018)
- **Research Fellowship** at the **Indian Institute of Technology Guwahati (India)** under the supervision of Prof. Nanda Kishore (Jan 2014 – Jul 2018)
- Won **Chemical Funda** competition at **SLIET**, India (2012)
- Scored **All India 46$^{th}$** rank in **SET** examination (2010)

## Professional Affiliations

- **Indian Institute of Chemical Engineers** (Membership no.: LAM-62040)

## Personal Details

**Father's Name** : Late Mr. Krishna Kumar Verma

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| **Mother's Name** | : | Mrs. Vimla Devi |
| **Date of Birth** | : | 3rd July 1993 |
| **Marital Status** | : | Single |
| **Nationality/Religion** | : | Indian/Hinduism |
| **Interest & Hobbies** | : | Gardening, Watching Movies, Story Writing, etc. |

## Publications

### International Refereed Journals

**2023**

**27)** Mohammad Saleheen, Osman Mamun, **Anand M. Verma**, Dia Sahsah, and Andreas Heyden, "Understanding the influence of solvents on the Pt-catalyzed hydrodeoxygenation of guaiacol", ***Journal of Catalysis***, 425, 212-232, 2023.

**26)** Anwin John, **Anand M. Verma**, M Shaneeth, and Ananth Govind Rajan, "Discovering a Single-Atom Catalyst for $CO_2$ Electroreduction to $C_1$ Hydrocarbons: Thermodynamics and Kinetics on Aluminum-Doped Copper", ***ChemCatChem***, accepted (in press) 2023.

**2022**

**25)** Ankit K. Verma, **Anand M. Verma**, and Ananth Govind Rajan, "Theoretical understanding of electrochemical phenomena in 2D electrode materials", ***Current Opinion in Electrochemistry***, 36, 101116, 2022.

**24) Anand M. Verma**, Laura Laverdure, Marko M. Melander, and Karoliina Honkala, "Mechanistic Origins of the pH Dependency in Au-Catalyzed Glycerol Electro-oxidation: Insight from First-Principles Calculations", ***ACS Catalysis***, 12, 662-675, 2022.

**2021**

**23) Anand M. Verma**, Karoliina Honkala, and Marko M. Melander, "Computational Screening of Doped Graphene Electrodes for Alkaline $CO_2$ Reduction", ***Frontiers in Energy Research***, 8, 606742 (1-15), 2021.

**22) Anand M. Verma**, Satya Pal Singh, and R P Ojha, "Quantum Chemical Study of Gas-Phase Reactions of Isoprene with OH Radicals Producing Highly Oxidized Second-Generation Products", ***Journal of Molecular Modelling***, 27, 62(1-10), 2021.

**2019**

**21) Anand M. Verma** and Nanda Kishore, "First-Principles Study on Gas-Phase Decomposition of Bio-oil Oxygenated Compounds over Palladium Catalyst Surface", ***Physical Chemistry Chemical Physics***, 21, 22320-22330, 2019.

**20)** Mohammad Saleheen, **Anand M. Verma**, Osman Mamun, Jianmin Lu, and Andreas Heyden, "Investigation of Solvent Effects on the Hydrodeoxygenation of Guaiacol over Ru Catalysts", ***Catalysis Science & Technology***, 9, 6253-6273, 2019.

**19)** Kushagra Agrawal, **Anand M. Verma**, and Nanda Kishore, "DFT Investigation on Thermochemical Analyses of Conversion of Xylose to Linear Alkanes in Aqueous Phase", ***Journal of Molecular Graphics and Modelling***, 90, 199-209, 2019.

**18)** Kushagra Agrawal, **Anand M. Verma**, and Nanda Kishore, "Thermochemical Conversion of Guaiacol in

Aqueous Phase by Density Functional Theory", ***ChemistrySelect,*** 4, 6013-6025, 2019.

**17)** Minttu M. Kauppinen, Ville Korpelin, **Anand M. Verma**, Marko M. Melander, and Karoliina 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.

## 2018

**16) Anand M. Verma**, Kushagra Agrawal, Harshal D. Kawale, and Nanda Kishore, "Production of Toluene by Decomposition of 2-Hydroxy-6-methylbenzaldehyde: A DFT Study", ***ChemistrySelect***, 3, 12279-12288, 2018.

**15) Anand M. Verma**, Harshal D. Kawale, Kushagra Agrawal, and Nanda Kishore, "Quantum Chemical Study on Gas Phase Pyrolysis of p-Isopropenylphenol", ***Journal of Molecular Graphics and Modelling***, 81, 134-145, 2018.

**14) Anand M. Verma**, Kushagra Agrawal, Harshal D. Kawale, and Nanda Kishore, "Quantum Chemical Study on Gas Phase Decomposition of Ferulic Acid", ***Molecular Physics***, 116, 1895-1907, 2018.

**13) Anand M. Verma**, Kushagra Agrawal, and Nanda Kishore, "Binding of Phenolic Model Compounds with Noble Metal Doped Graphene Sheets", ***Computational and Theoretical Chemistry***, 1134, 37-46, 2018.

**12) Anand M. Verma**, Kushagra Agrawal, and Nanda Kishore, "Computational Study on Ring Saturation of 2-Hydroxybenzaldehyde Using Density Functional Theory", ***ACS Omega***, 3, 8546-8552, 2018.

**11) Anand M. Verma** and Nanda 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.

**10) Anand M. Verma**, Kushagra Agrawal, and Nanda Kishore, "Elucidation of Novel Mechanisms to Produce Value-Added Chemicals from Vapour Phase Conversion of Ferulic Acid", ***Theoretical Chemistry Accounts***, 137, 122(1-10), 2018.

**9) Anand M. Verma** and Nanda Kishore, "Decomposition Mechanisms of Acetic Acid over Ru and Ru/MgO Clusters under DFT Framework", ***Chemical Physics Letters***, 711, 156-165,2018.

## 2017

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

**7) Anand M. Verma** and Nanda Kishore, "Gas Phase Conversion of Eugenol into Various Hydrocarbons and Platform Chemicals", ***RSC Advances***, 7, 2527-2543, 2017.

**6) Anand M. Verma** and Nanda Kishore, "Molecular Modelling Approach to Elucidate the Thermal Decomposition Routes of Vanillin", ***New Journal of Chemistry***, 41, 8845-8859, 2017.

**5) Anand M. Verma** and Nanda Kishore, "Thermochemistry Analyses for the transformation of C6 Glucose compound into C9, C12, and C15 Alkanes using Density Functional Theory", ***Molecular Physics***, 115, 413-423, 2017.

**4) Anand M. Verma** and Nanda Kishore, "DFT Study on Gas Phase Hydrodeoxygenation of Guaiacol by Various Reaction Schemes", ***Molecular Simulation***, 43, 141-153, 2017.

**3) Anand M. Verma** and Nanda Kishore, "Production of Benzene from 2-Hydroxybenzaldehyde by Various Reaction Paths using IRC Calculations within a DFT framework", ***ChemistrySelect***, 2, 1556-1564, 2017.

**2) Anand M. Verma** and Nanda Kishore, "Platinum Catalysed Hydrodeoxygenation of Guaiacol in Illumination of Cresol Production: A Density Functional Theory Study", ***Royal Society Open Science***, 4, 170650(1-12), 2017.

**2016**

**1) Anand M. Verma** and Nanda Kishore, "DFT Analyses of Reaction Pathways and Temperature Effects on various Guaiacol Conversion Reactions in Gas Phase Environment", ***ChemistrySelect***, 1, 6196-6205, 2016.

## Book Chapters

1) **Anand M. Verma** and Nanda Kishore, "A Succinct Review on the Upgradation of Lignin Derived Bio-Oil Model Components", ***Sustainable Energy Technology and Policies***, Springer, 2018.
2) **Anand M. Verma** and Nanda Kishore, "Current Advances in Bio-oil Upgrading: A Brief Discussion", ***Sustainable Energy Technology and Policies***, Springer, 2018.

## Conferences/Posters/Proceedings

1) **Anand M. Verma**, ***NAMMA Psi-K workshop***, JNCASR and IISc Bengaluru, July 2023, India. **(Attendee)**
2) **Anand M. Verma**, ***IISc Chemical Engineering Symposium (ICES) and Alumni Meet***, IISc Bengaluru, June 2023, India. **(Attendee)**
3) **Anand M. Verma** and Ananth Govind Rajan, "First-principles investigations on thermocatalytic $CO_2$ reduction to various $C_1$-based products", ***ChemE 75 Symposium***, IISc Bengaluru, December 2022, India. **(Talk)**
4) **Anand M. Verma**, ***Shell AI Conference***, September 2022, Hotel Taj Bangalore, India. **(Attendee)**
5) **Anand M. Verma** and Ananth Govind Rajan, "Using Density Functional Theory and Machine Learning to predict Catalysts for Thermochemical $CO_2$ Conversion to 1-Butanol", ***Young Researchers' Symposium 2022***, IISc Bengaluru, April 2022, India. **(Poster)**
6) **Anand M. Verma**, ***APS Satellite Meeting***, March 2022, International Center for Theoretical Sciences, Bengaluru, India. **(Attendee)**
7) **Anand M. Verma**, ***Nanoscience Days***, October 2020, University of Jyväskylä, Finland. **(Attendee)**
8) **Anand M. Verma**, "First-Principles Study on Water Dissociation Reaction over Zirconia-Supported Pt and Rh Interfacial Sites", ***Computational Chemistry Days***, August 2019, University of Eastern Finland, Kuopio, Finland. **(Talk)**
9) **Anand M. Verma**, "Interfacial Water Dissociation over Globally Optimized $ZrO_2$ Supported Rh and Pt Clusters: A DFT Perspective", ***Nanoscience Days***, October 2019, University of Jyväskylä, Finland. **(Poster)**
10) **Anand M. Verma** and Nanda Kishore, "Kinetics of Decomposition Reactions of Acetic Acid using DFT Approach", ***The Open Journal of Chemical Engineering*** **(Invited Contribution)**, 12, 14-23, 2018.
11) **Anand M. Verma**, Kushagra Agrawal, and Nanda Kishore, "Gas Phase Kinetic Investigations of Decomposition of Salicylaldehyde over Pd(111) Catalyst Surface", ***REFLUX***, March 2018, IIT Guwahati, India. (Secured **1st position**). **(Talk)**
12) Kushagra Agrawal, **Anand M. Verma**, and Nanda Kishore, "Elucidating the Production of Vanillin from

Ferulic Acid using DFT", ***Research Conclave***, March 2018, IIT Guwahati, India. **(Talk)**

13) **Anand M. Verma** and Nanda Kishore, "DFT Study on Hydrogenation Reaction of Acetaldehyde to Ethanol in Gas and Water Phase", ***ICRTET***, January 2016, India. **(Talk)**

14) **Anand M. Verma** and Nanda Kishore, "DFT Study on Hydrogenation Reaction of Acetaldehyde to Ethanol in Gas and Water Phase", ***International Journal of Research in Engineering and Technology*** **(Invited Contribution)**, 5, 53-57, 2016.

15) **Anand M. Verma** and Nanda Kishore, "DFT Study on Hydrogenation Reaction of 1-hydroxypropan-2-one", ***30th Indian Engineers Congress, 21st Century Engineering: Make in India Pathway***, December 2015, India. **(Talk)**

**16) Anand M. Verma** and Nanda Kishore, "Theoretical comparison of DFT functional for the decomposition reaction of acetic acid", ***SCHEMCON***, Sep 2015, Pune, India. **(Talk)**

**17) Anand M. Verma** and Nanda Kishore, "DFT Study on Kinetics of Decomposition Reaction of trans-Methyl Nitrite", ***CHEMCON***, December 2015, India. **(Talk)**

## Workshops

1) **Anand M. Verma**, "Practical Machine Learning: GPU Edition!", ***CSC Finland***, October 2020, Finland.
2) **Anand M. Verma**, "Workshop on Theory, Applications, and Tools for Multiscale Kinetic Modeling", ***Laboratory of Catalysis and Catalytic Processes***, July 2020, Italy.
3) **Anand M. Verma**, "Spring School on Computational Chemistry 2020", ***CSC Finland***, January 2020, Finland.
4) **Anand M. Verma**, "A Workshop on Gaussian 09 Software Package", Pune 2014, India.

## References

| Details | Referee 1 | Referee 2 | Referee 3 |
|---|---|---|---|
| **Name of Referee** | Prof. Ananth Govind Rajan | Prof. Nanda Kishore | Prof. Karoliina Honkala |
| **Organisation** | Indian Institute of Science, Bengaluru, India | Indian Institute of Technology Guwahati, India | University of Jyväskylä, Finland |
| **Designation** | Assistant Professor | Professor | Professor |
| **Relationship with Applicant** | Postdoc Supervisor | PhD Supervisor | Previous Postdoc Supervisor |
| **E-mail ID** | ananthgr@iisc.ac.in | nkishore@iitg.ac.in | karoliina.honkala@jyu.fi |
| **Phone number** | +91-8022933702 | +91-3612582276 | +358-408053686 |

## Declaration

I hereby declare that the information furnished above is true to the best of my knowledge and belief.

Anand Mohan Verma

**Date: August 23, 2023** **(Anand Mohan Verma)**