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Summary

I am a PhD student at Wageningen University & Research (WUR), the Netherlands. I am enthusiastic about coupling computational tools with chemical/physical/materials science knowledge to gain insights into some of the most fundamental processes. Specifically, in my PhD, I am studying fundamental reactions involved in the conversion of biobased-feedstock to platform chemicals for biofuels. The goal is to design cheap-and-efficient catalysts for biomass conversion. For this, I use knowledge of chemical/physical science and mathematical modelling to run computer simulations. For such simulations, the underlying theories are the widely used computational approaches like density functional theory (DFT), *ab initio* molecular dynamics (AIMD), microkinetic modelling (MKM), etc. I am also interested in learning to accelerate these approaches by the means of machine learning (ML) and artificial intelligence (AI) tools. Apart from research, I play, and intensively follow, football, and I am also learning to play piano & guitar.

Research interests

Computational materials science, surface science, heterogeneous catalysis, and application of data science & machine learning in catalysis design and discovery.

Research experience

Oct 2020 - Present	Doctoral Student at Wageningen University & Research (WUR), The Netherlands Supervisors: Prof. Han Zuilhof & Prof. Harry Bitter & Prof. Guanna Li Biobased Chemistry and Technology (BCT) & Organic Chemistry(ORC), WUR Topic: Multiscale modelling of transition metal carbide catalysts for biomass conversion.
May 2019 - May 2020	Master Thesis Student- Advisors: Prof. Michele Casula and Prof. Prasenjit Ghosh Université Pierre et Marie Curie (UPMC), (IMPMC) - Sorbonne University, France Topic: Magnetic properties of narrow zigzag graphene nanoribbons from *ab initio* calculations.
August 2018 - May 2019	Research Intern- Advisor: Prof. Prasenjit Ghosh, Department of Physics Indian Institute of Science Education and Research Pune, India Topic: Electronic structure calculations of solid materials using Quantum ESPRESSO.
May 2018 – July 2018	Summer Research Intern- Advisor: Prof. Eluvathingal D. Jemmis Indian Institute of Science, Department of Inorganic and Physical Chemistry, India Topic: Theoretical study of isonitrile coupling mediated by allenic diborenes.

Publications

- **Raghavendra Meena**, Guanna Li, and Michele Casula. *Ground-state properties of the narrowest zigzag graphene nanoribbon from quantum Monte Carlo and comparison with density functional theory.* J. Chem. Phys. 156, 084112 **(2022)**.
- Sagar Ghorai, **Raghavendra Meena**, Anju P. Joseph, and Eluvathingal D. Jemmis. *Comparison of RNC Coupling and CO Coupling Mediated by Cr–Cr Quintuple Bond and B–B Multiple Bonds: Main Group Metallomimetics.* The Journal of Physical Chemistry A **2021** 125 (33), 7207-7216.

Skills

Modules	GAUSSIAN, QuantumESPRESSO, TurboRVB (for QMC methods), VASP, CP2K, ASE, and Blender.
Languages	Basic: MATLAB, C++, and bash scripting Intermediate: Python, and LaTeX
Others	1) More than 4 years of experience in using supercomputing resources. 2) Linux/macOS/Windows environment.

Education

Oct 2020– Present	PhD, Theoretical Chemistry Wageningen University & Research, The Netherlands
May 2019– May 2020	Master's thesis, Computational Materials Science Université Pierre et Marie Curie (UPMC, Sorbonne Université), Paris, France
Aug 2015– April 2020	BS-MS Dual Degree, Chemistry and Physics Indian Institute of Science Education and Research, Pune, Maharashtra, India

Grants/Awards/Scholarships

- Computational budget granted by NWO SURFsara on Snellius machine (**1 x 500,000 SBUs and 2 x 1,000,000 SBUs**).
- Erasmus+ inter-institutional credit mobility fellowship awarded by the European Union, **2019-2020**.
- INSPIRE (Innovation in Science Pursuit for Inspired Research) Scholarship awarded by the Department of Science and Technology, India, **2015-2020**.
- National Talent Search Scholarship (NTSE) Scholarship awarded by National Council for Educational Research and Training (NCERT), India, **July 2013**.

Certifications

- Oral presentations at NWO CHemistry As INnovativing Science (NWO-CHAINS)(**2022**; The Netherlands).
- Poster presentations at International Conference on Theoretical Aspects of Catalysis (ICTAC) (**June 2022**; Lyon, France.), Netherlands' Catalysis and Chemistry Conference (N3C) (**May 2022**; The Netherlands).
- Attendance at CECAM MolSim "*Understanding Molecular Simulation*" course (**2023**), Han-sur-Lesse winter school for theoretical & computational chemistry (**2021)**, Paris International School on Advanced Computational Materials Science (PISACMS) (**2021**), and International Conference on Electrocatalysis for Energy Applications and Sustainable Chemicals (EcoCat) (**2020**) (online).

Teaching & Supervision

- Supervised 2 MSc Major & 1 MSc Minor thesis, and a BSc practical course in Bio-Organic Chemistry for Life Sciences.
- TA in the following courses: Computer modeling of biomolecules, Biofunctional food ingredients, structure & reactivity.