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Research interests

Computational materials science, surface science, heterogeneous catalysis, and application of data science & machine learning for catalyst 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 Topic: Multiscale modelling of transition metal carbide catalysts for biomass conversion. Application of density functional theory (DFT), microkinetic modelling (MKM), and molecular dynamics (MD) for designing transition metal carbide catalysts.
May 2019 - May 2020	Master Thesis Student at Sorbonne University, France Supervisors: Prof. Michele Casula and Prof. Prasenjit Ghosh Topic: Magnetic properties of narrow zigzag graphene nanoribbons (zGNRs) from *ab initio* calculations. Use of DFT and Quantum monte carlo (QMC) to study the magnetic properties of zGNRs, and benchmarking of DFT functionals with more accurate QMC results.
August 2018 - May 2019	Research Intern at Indian Institute of Science Education and Research Pune, India Supervisor: Prof. Prasenjit Ghosh Topic: Electronic structure calculations of solid materials using Quantum ESPRESSO. Application of DFT for calculating electronic band structure, and density of states.
May 2018 – July 2018	Summer Research Intern at Indian Institute of Science, India Supervisor: Prof. Eluvathingal D. Jemmis and Dr. Sagar Ghorai Topic: Theoretical study of isonitrile coupling mediated by allenic diborenes. Use of DFT for studying the reaction mechanism of isonitrile coupling mediated by allenic diborenes, and its comparison with transition metal complexes.

Publications (GoogleScholar)

- **Raghavendra Meena**, Johannes Hendrik Bitter, Han Zuilhof, Guanna Li. *Toward the Rational Design of More Efficient Mo_2C Catalysts for Hydrodeoxygenation–Mechanism and Descriptor Identification.* ACS Catalysis (**2023**), 13, 13446–13455.
- Hao Zhang, Aleksei Bolshakov, **Raghavendra Meena**, Gustavo A. Garcia, A. Lulian Dugulan, Alexander Parastaev, Guanna Li, Emiel J. M. Hensen, and Nikolay Kosinov. *Revealing Active Sites and Reaction Pathways in Methane Non-Oxidative Coupling over Iron-Containing Zeolite.* Angew. Chem. Int. Ed. (**2023**), e202306196.
- **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)**. Publication from the work done during Masters' thesis.
- 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. Publication from the work done during a research internship.

Skills

Modules	**DFT**: GAUSSIAN, Quantum ESPRESSO, VASP, ASE; **QMC**: TurboRVB; **MD/Metadynamics**: CP2K, VASP; **Molecule rendering/visualization**: Blender, VMD, and Materials Studio.
Languages	Basic: MATLAB, and C++; Intermediate: Python, bash scripting, and LaTeX.
Others	1) More than 6 years of experience using supercomputing resources. 2) Linux/MacOS/Windows environment.

Education

Oct 2020– Sept 2024	PhD, Theoretical Chemistry & Computational Chemistry Wageningen University & Research, The Netherlands
May 2019– May 2020	Master's thesis (part of BS-MS Dual Degree), 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 3 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, **2013-2015**.

Certifications

- Oral presentations at CHemistry As INnovating Science (CHAINS) **2022** and Netherlands's Chemistry and Catalysis Conference (NCCC) **2023**.
- 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 3 MSc major thesis, 1 MSc minor thesis, 2 BSc thesis, and a BSc practical course in Bio-Organic Chemistry for Life Sciences.
- Teaching assistant in the following courses: Computer modelling of biomolecules, Biofunctional food ingredients, structure & reactivity.