Raj Kumar Paudel

Ph.D., Postdoctoral Research Fellow

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Summary

Highly motivated Postdoctoral Research Fellow with expertise in quantum-mechanics-based computational techniques, particularly Density Functional Theory (DFT) and the Semi-Empirical Pseudopotential Method (SEPM). Focused on developing and applying advanced computational frameworks to investigate electronic and optical properties of emerging quantum materials, including 2D materials (graphene, TMDCs), nanos-tructures, and molecular systems (fullerenes). Key interests include exciton physics in 2D layer materials and method development for efficient, accurate material simulations.

Education

Sep 2016 – Jul Ph.D. in Physics, Taiwan International Graduate Program (TIGP), Academia Sinica & 2023 National Central University, Taipei, Taiwan Dissertation: Novel Computational Approaches for Electronic Structure of Two-Dimensional Materials using the Semi-Empirical Pseudopotential Method Supervisor: Prof. Yia-Chung Chang
 Oct 2006 – Jun M.Sc. in Physics, Central Department of Physics, Tribhuvan University, Kirtipur, 2009 Nepal

Research Experience

Aug 2023 – Postdoctoral Research Fellow, RCAS, Academia Sinica, Taipei, Taiwan
 Present O Developing and applying SEPM and DFT to investigate the electronic and optical properties of quantum materials (TMDCs, fullerenes, graphene).

- \circ Modeling exciton binding energies and optical responses in bilayer MoS₂ and WSe₂.
- \odot Investigating charge transfer mechanisms in C₆₀ molecular assemblies.

○ Supervisor: Prof. Yia-Chung Chang

- Sep 2016 Jul Ph.D. Researcher, Academia Sinica & National Central University (TIGP Program), 2023 Taipei, Taiwan
 - Developed and implemented the Semi-Empirical Pseudopotential Method (SEPM) for 2D materials.
 - Applied SEPM to study electronic structures of graphene, armchair graphene nanoribbons, and monolayer TMDCs.
 - O Parameterized local and non-local pseudopotentials for various material systems.

○ Supervisor: Prof. Yia-Chung Chang

Technical Skills

Computational Methods

- Density Functional Theory (DFT)
- Semi-Empirical Pseudopotential Method (SEPM)
- Exciton Physics & Dynamics Modeling

Programming

Python (NumPy, SciPy, Matplotlib)

- Fortran, C
- Bash Scripting
- Version Control (Git, GitHub)

Software & Environments

- Local Planar Basis DFT package
- Quantum ESPRESSO, VASP (DFT Packages)
- High-Performance Computing (HPC) Environments

Material Systems

- 2D Materials (Graphene, TMDCs)
- \odot Graphene Nanoribbons, Fullerenes (C₆₀)
- Exciton Physics in Bilayer TMDCs

Languages

- Nepali (Native)
- English (Fluent)
- Chinese (Basic)

Awards and Honors

- Taiwan International Graduate Program (TIGP) Scholarship for PhD (Sep 2016 Jul 2023)
- NAST Research Grant for Master's Thesis, Nepal Academy of Science and Technology (Oct 2008)

Publications

Preprints

- Paudel, R. K., Ren, C.-Y., & Chang, Y.-C. (2025). Semiempirical Pseudopotential Method for Transitional-Metal Dichalcogenides (Submitted to Physical Review Applied).
- Cha, S., Xu, Z., Ouyang, T., Yao, H., Paudel, R. K., Taniguchi, T., Watanabe, K., Joe, A. Y., Chang, Y.-C., Gabor, N. M., & Lui, C. H. (2025). 2P Interlayer Exciton Revealed by Hybridization in Bilayer MoS₂. (Submitted to Nature Physics)
- Tianyi Ouyang, Erfu Liu, Soonyoung Cha, Raj Kumar Paudel, Yiyang Sun, Zhaoran Xu, Takashi Taniguchi, Kenji Watanabe, Nathaniel M. Gabor, Yia-Chung Chang, Chun Hung Lui. Brightening Interlayer Excitons by Electric-Field-Driven Hole Transfer in Bilayer WSe₂ (2025) submitted to Physical Review Letters

Peer-Reviewed Journal Articles

- Paudel, R. K., Ren, C.-Y., & Chang, Y.-C. (2023). Semi-Empirical Pseudopotential Method for Graphene and Graphene Nanoribbons. *Nanomaterials*, 13(14), 2066.
- Ren, C.-Y., Paudel, R. K., & Chang, Y.-C. (2023). Density Functional Theory for Buckyballs within Symmetrized Icosahedral Basis. *Nanomaterials*, 13(13), 1912.

Conference Presentations

- Paudel, R. K. (2024). Semi-Empirical Pseudopotential Methods for Low-Dimensional Materials. *MRS Spring Meeting*, Seattle, WA, USA.
- Paudel, R. K., Ren, C.-Y., & Chang, Y.-C. (2023). Semi-Empirical Pseudopotential Method for Graphene and Armchair Graphene Nanoribbons. *CCP2023 - 34th IUPAP Conference on Computational Physics*, Kobe, Japan.
- Paudel, R. K. (2022). Development of Semi-Empirical Pseudopotential Method for Two Dimensional Materials. 20th Workshop on First-Principles Computational Materials Physics, Kaohsiung, Taiwan.

Professional Affiliations

Memberships

- Member, Taiwan Physical Society (TPS)
- Member, American Physical Society (APS)
- Life Member, Nepal Physical Society (NPS)

References

- Prof. Y.-C. Chang Distinguished Research Fellow, RCAS Academia Sinica, Taiwan ychang@gate.sinica.edu.tw
- Prof. C.-Y. Ren
 Professor, Dept. of Physics
 National Kaohsiung Normal University (NKNU), Taiwan
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