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Raj Kumar Paudel

Ph.D., Postdoctoral Research Fellow

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), nanostructures, and molecular systems (fullerenes). Key interests include exciton physics in 2D heterostructures and method development for efficient, accurate material simulations.

Education

Sep 2016 – Jul 2023 **Ph.D. in Physics**, *Taiwan International Graduate Program (TIGP), Academia Sinica & 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 2009 **M.Sc. in Physics**, *Central Department of Physics, Tribhuvan University*, Kirtipur, Nepal

Oct 2002 – Sep 2006 **B.Sc. in Physics (Major)**, *Tribhuvan University*, Kathmandu, Nepal

Research Experience

Aug 2023 – Present **Postdoctoral Research Fellow**, *RCAS, Academia Sinica*, Taipei, Taiwan
- Developing and applying SEPM and DFT to investigate the electronic and optical properties of quantum materials (TMDCs, fullerenes, graphene).
- Modeling exciton binding energies, dynamics, and optical responses in monolayer and bilayer TMDCs.
- Investigating charge transfer mechanisms in C_{60} molecular assemblies.

Supervisor: Prof. Yia-Chung Chang

Sep 2016 – Jul 2023 **Ph.D. Researcher**, *Academia Sinica & National Central University (TIGP Program)*, 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.
- 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)
- Many-Body Perturbation Theory (GW, BSE)
- Exciton Physics & Dynamics Modeling

Programming

- Python (NumPy, SciPy, Matplotlib)
- Fortran, C
- Bash Scripting
- Machine Learning
- 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)
- Graphene Nanoribbons, Fullerenes (C_{60})
- 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)
- Merit Student, Central Department of Physics, Tribhuvan University (2007)
- Full M.Sc. Scholarship, Tribhuvan University (Oct 2006 – Jun 2009)

Publications

(Complete list at Google Scholar or personal website.)

Preprints

- Paudel, R. K., Ren, C.-Y., & Chang, Y.-C. (2025). Semiempirical Pseudopotential Method for Transitional-Metal Dichalcogenides. arXiv:2506.11360. (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 MoS_2. arXiv:rs-6734783.(Submitted to Nature Physics)
- Ouyang, T., Liu, E., Cha, S., **Paudel, R. K.**, Sun, Y., Xu, Z., Taniguchi, T., Watanabe, K., Gabor, N. M., Chang, Y.-C., & Lui, C. H. (2025). Brightening Interlayer Excitons by Electric-Field-Driven Hole Transfer in Bilayer WSe_2. (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

Oral Presentation

- Paudel, R. K. (2022). Development of Semi-Empirical Pseudopotential Method for Two Dimensional Materials. *20th Workshop on First-Principles Computational Materials Physics*, Kaohsiung, Taiwan.

Poster 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.

Professional Affiliations

Memberships

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

References

Prof. Yia-Chung Chang
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