

Raj Kumar Paudel

Ph.D., Postdoctoral Research Fellow

Summary

Computational materials physicist with expertise in Density Functional Theory (DFT), the Semi-Empirical Pseudopotential Method (SEPM), and quantum transport simulations. Experienced in developing and applying computational frameworks to study the electronic, optical, and transport properties of low-dimensional quantum materials, including graphene, transition-metal dichalcogenides (TMDCs), fullerene systems, and van der Waals heterostructures. Recent work focuses on non-equilibrium Green's function (NEGF)-based quantum transport in molecule-functionalized 2D systems such as F4TCNQ-doped graphene, as well as exciton physics in bilayer and twisted TMDCs, interlayer coupling effects, and scalable simulations for nano-electronic devices.

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 2025 – Present **Postdoctoral Research Fellow**, *Department of Physics, National Cheng Kung University (NCKU)*, Tainan, Taiwan
- Developing quantum transport methods for mesoscopic and low-dimensional devices using non-equilibrium Green's function (NEGF) formalism.
 - Investigating charge transfer and transport in molecule-functionalized 2D materials, including F4TCNQ-doped graphene.
 - Performing large-scale computational simulations for nanoelectronic and quantum-material systems.
- Supervisor: Prof. Ming-Hao Liu*
- Aug 2023 – Jul 2025 **Postdoctoral Research Fellow**, *Research Center for Applied Sciences (RCAS), Academia Sinica*, Taipei, Taiwan
- Developed and applied SEPM and DFT methods to investigate electronic and optical properties of quantum materials, including TMDCs, graphene, and fullerene systems.
 - Modeled exciton binding energies, interlayer excitons, and optical responses in monolayer and bilayer TMDCs.
 - Investigated charge-transfer mechanisms in C₆₀ molecular assemblies and low-dimensional materials.
- 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 low-dimensional materials.
- Applied SEPM to study the electronic structures of graphene, armchair graphene nanoribbons, and monolayer TMDCs.
- Parameterized local and nonlocal pseudopotentials for multiple material systems.

Supervisor: Prof. Yia-Chung Chang

Technical Skills

Methods Density Functional Theory (DFT), Semi-Empirical Pseudopotential Method (SEPM), Quantum Transport Simulations (NEGF), Many-Body Perturbation Theory (GW/BSE), Exciton Physics and Optical Response Modeling

Programming Fortran, Python, C, Bash, NumPy, SciPy, Matplotlib, Git/GitHub

Software Quantum ESPRESSO, SIESTA, VASP, Wannier90, VESTA, XCrySDen, HPC Environments

Material Systems Graphene, Graphene Nanoribbons, TMDCs, Fullerenes, van der Waals Heterostructures, Bilayer Systems, organic molecule doped graphene.

Languages Nepali (Native), English (Fluent), Chinese (Basic)

Awards and Honors

- Taiwan International Graduate Program (TIGP) Scholarship for Ph.D. Studies (2016–2023)
- NAST Research Grant for Master's Thesis, Nepal Academy of Science and Technology (2008)
- Merit Student Award, Central Department of Physics, Tribhuvan University (2007)
- Full M.Sc. Scholarship, Tribhuvan University (2006–2009)

Publications

Complete publication list available at [Google Scholar](#) and [personal website](#).

Preprints and Submitted Articles

- 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. Hybridization-revealed interlayer 2p exciton state in bilayer MoS₂. [Research Square preprint](#). accepted to **Nature Physics**.

Peer-Reviewed Journal Articles

- **Paudel, R. K.**, Ren, C.-Y., & Chang, Y.-C. Semi-empirical Pseudopotential Method for Monolayer Transition Metal Dichalcogenides, *Computer Physics Communications*, **327**, 110240 (2026) DOI: <https://doi.org/10.1016/j.cpc.2026.110240>
- 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. Brightening Interlayer Excitons by Electric-Field-Driven Hole Transfer in Bilayer WSe₂. *Physical Review Letters* **136**, 096903 (2026) DOI: <https://journals.aps.org/prl/abstract/10.1103/mjhj-83wc>
- **Paudel, R. K.**, Ren, C.-Y., & Chang, Y.-C. Semi-Empirical Pseudopotential Method for Graphene and Graphene Nanoribbons. *Nanomaterials* **13**(14), 2066. (2023) DOI: <https://doi.org/10.3390/nano13142066>

- Ren, C.-Y., **Paudel, R. K.**, & Chang, Y.-C. Density Functional Theory for Buckyballs within Symmetrized Icosahedral Basis. *Nanomaterials* **13**(13), 1912. (2023)
DOI: <https://doi.org/10.3390/nano13131912>

Conference Presentations

Oral Presentations

- **Paudel, R. K.**, Ren, C.-Y., & Chang, Y.-C. Semiempirical Pseudopotential Method for Transition-Metal Dichalcogenides. *CCP2025 – 36th IUPAP Conference on Computational Physics*, Oakridge, USA, (2025 Virtual)
- Ouyang, T., Liu, E., Cha, S., **Paudel, R. K.**, et al. Brightening Interlayer Excitons by Electric-Field-Driven Hole Transfer in Bilayer WSe_2 . *23rd Workshop on First-Principles Computational Materials Physics* (2025), Kaohsiung, Taiwan.
- **Paudel, R. K.** Development of Semi-Empirical Pseudopotential Method for Two-Dimensional Materials. *20th Workshop on First-Principles Computational Materials Physics*, Kaohsiung, Taiwan. (2022)

Poster Presentations

- Cha, S., Xu, Z., Ouyang, T., Yao, H., **Paudel, R. K.**, et al. Hybridization-revealed interlayer 2p exciton state in bilayer MoS_2 . *26th Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-26)*, RIKEN, Japan, (2025).
- **Paudel, R. K.** Semi-Empirical Pseudopotential Methods for Low-Dimensional Materials. *MRS Spring Meeting*, Seattle, WA, USA, (2024).
- **Paudel, R. K.**, Ren, C.-Y., & Chang, Y.-C. Semi-Empirical Pseudopotential Method for Graphene and Armchair Graphene Nanoribbons. *CCP2023 – 34th IUPAP Conference on Computational Physics*, Kobe, Japan. (2023)

Professional Affiliations

Memberships

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

References

Prof. Yia-Chung Chang

Distinguished Research Fellow
Research Center for Applied Sciences (RCAS)
Academia Sinica, Taipei, Taiwan
Adjunct Professor, Department of Physics
National Cheng Kung University (NCKU)
Tainan, Taiwan
ychang@gate.sinica.edu.tw

Prof. Ming-Hao Liu

Professor, Department of Physics
National Cheng Kung University (NCKU)
Tainan, Taiwan
minghao.liu@phys.ncku.edu.tw