

## Contact

601-466-6997 (Mobile)  
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## Top Skills

Computational Physics  
Materials Modeling  
Density Functional Theory  
Parallel Computing  
Machine Learning tools

## Certifications

- Professional Development (Professionals in Preparation) Foundational-Level
- Machine Learning Foundations: A Case Study Approach
- IBM Quantum Challenge
- Deep Learning Specialization
- Python for Data Science and Machine Learning Bootcamp

## Publications

- *Ab Initio* Hydrogen Dynamics and the Morphology of Voids in Amorphous Silicon
- Disorder by design: A data-driven approach to amorphous semiconductors without total-energy functionals
- *Ab initio* density-functional studies of 13-atom Cu and Ag clusters
- Atomistic simulation of nearly defect-free models of amorphous silicon: An information-based approach
- Structure of transition metal clusters: A force-biased Monte Carlo approach
- Information-driven inverse approach to disordered solids: Applications to amorphous silicon
- Structural properties of transition-metal clusters via force-biased Monte Carlo and *ab initio* calculations: A comparative study

# Dil K. Limbu

Ph.D. Scholar in Computational Physics | Computational Materials Science  
Hattiesburg, MS 39401, USA

## Summary

Experienced and highly self-motivated Ph.D. Scholar seeking to deepen knowledge of material modeling by completing independent/collaborative research projects focused on complex functional materials. Experienced using density functional theory calculations for structural modeling and exploring the relationship in material phenomena, with expertise in Fortran/ Python programming, High-Performance Computing (HPC), and machine learning algorithms in current research in materials science.

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## Experience

The University of Southern Mississippi  
5 years 10 months

Graduate Research Assistant  
June 2016 – May 2021 (5 years 0 month)  
118 College Drive, #5046 Hattiesburg, MS 39406

- Force-biased and *ab initio* modeling of transition metal clusters: Developed a force-biased Monte Carlo (FMC) optimization method for structural modeling of transitional metal clusters
- Disorder by Design: Data-Driven Approaches to Complex Materials: Developed a multi-objective optimization approach to map the structure determination via inversion of diffraction data in conjunction with a few structural constraints for amorphous solids
- *Ab initio* Hydrogen Dynamics and Morphology of Voids in *a*-Si: Characterized H-dynamics near the voided surface of high-quality *a*-Si/*a*-Si:H models from *ab initio* molecular-dynamics simulations

Graduate Teaching Assistant  
August 2015 - May 2021 (5 years 10 months)  
118 College Drive, #5046 Hattiesburg, MS 39406

- Courses taught: Introductory Physics Laboratory 111L/112L, General Astronomy 111L/112L, General Physics with Calculus 201L
- Conducted timely setup, storage, and maintenance of laboratory equipment

## Programming Language

- Fortran
- Python
- C/C++
- CUDA
- MPI/OpenMP

## Software Package

- VASP
- SIESTA
- NWChem
- RMCPProfile
- LAMMPS
- Matlab
- VMD
- Gnuplot
- grace
- Latex
- Xcrysden
- Jmol

## Operating system

- Linux (Ubuntu)
- Windows
- Unix

## Award and Honors

- Recognized for computational support in 2019 NSF-HBCU Summer School on Computational Modeling of Disordered Solids, (June 3–7, 2019), USM, Gulf Park Campus, Long Beach, MS
- Travel award for outstanding poster presentation in Susan A. Siltanen Graduate Student Research Symposium, (April 11, 2019), USM, Hattiesburg, MS
- Best Teacher Award, (2014), Shuvatara School, Lalitpur
- Merit-based Scholarship Award, (2004), Tribhuvan University

- Utilized email, phone and in-person meetings to answer questions and mentor struggling students
- Adhered to university requirements for student assignments, testing and grading of work

## Shuvatara School

### Science Teacher

September 2010 - June 2015 (4 years 10 months)

Lalitpur District, Nepal

- Adapted teaching methods and instructional strategies to promote learning in students of differing skill levels.
- Assessed student progress with course material through routine quizzes, final examinations, and standardized assessments.
- Managed consistent, learning-focused classroom environments by establishing and communicating clear objectives for all students.
- Met with parents and guardians to discuss student progress and areas for improvement.

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## Education

### The University of Southern Mississippi

PhD, Computational Science (Physics) · (June 2017 – May 2021)

### The University of Southern Mississippi

Master of Science - MS, Physics · (August 2015 – May 2017)

### Tribhuvan University, Nepal

Master of Science (M.Sc.), Physics · (December 2010)

### Tribhuvan University, Nepal

Bachelor of Science (B.Sc.), Physics, Computer Science · (March 2006)

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## Professional Membership

- Student member, American Physical Society (APS)
- Student member, Society of Physics Students (SPS)
- Student member, Material Research Society (MRS)
- Student member, American Ceramic Society (ACerS)
- Student member, Association of Nepali Physicists in America (ANPA)