Deep Arnold Gomes

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Research Profile

Computational condensed matter physicist specializing in defect physics electronic structure and structure dependent properties of low dimensional and oxide based materials. My research integrates first principles calculations with experimental validation to understand how curvature composition and local coordination geometry control defect energetics band edge behavior and catalytic activity. Experience spans DFT defect modeling phonons NEB reaction pathways and experimental work on magnetic critical behavior. Seeking PhD training at Penn State to work at the interface of computational prediction and nanoscale measurement especially with groups focused on defect driven phenomena in two dimensional and oxide systems.

Research Interests

Defects and dopants in low dimensional systems · First principles electronic structure · Curvature and strain effects · Oxide vacancy thermodynamics · Phonons and vibrational signatures · Single atom catalysis mechanisms · Magnetic critical behavior · Computational materials design with experimental validation

Education

MSc in Physics Condensed Matter and Materials Physics *June 2023 to January 2025*
Department of Physics University of Dhaka Bangladesh
GPA: 3.40 / 4.00
Thesis: *Electronic structure and defect effects in TiO2 based low dimensional systems*

BSc Honors in Physics *2018 to 2023*
Department of Physics University of Dhaka Bangladesh
CGPA: 3.57 / 4.00 (Perfect 4.00 in all experimental courses)

Research Experience

Research Fellow International Science Programme Uppsala University *2023 to 2026*
Soft Matter and Nanophysics Laboratory University of Dhaka

- Performed spin polarized DFT calculations using VASP for defect formation energetics charge localization band edge shifts and relaxation behavior in TiO2 nanotubes across more than fifty configurations.
- Identified that Cu atoms preferentially form surface clusters rather than substitutional defects producing a measured 0.3 eV band edge shift confirmed through UV visible spectroscopy.
- Demonstrated that curvature modifies defect stability and electronic structure showing 0.3 eV shifts in defect localization when moving from flat to curved oxide geometries.
- Computed phonon dispersion to reveal how confinement and doping alter vibrational signatures enabling direct experimental identification of defect configurations.
- Modeled Mn doped graphene using nudged elastic band methods showing activation barriers between 0.41 and 0.78 eV and revealing that local lattice relaxation can shift barriers by up to 0.37 eV.

- Established ligand field driven catalytic activity principles from Bader charge analysis providing design insight for single atom catalysts while avoiding metal leaching pathways.
- Integrated computational predictions with experimental UV visible spectroscopy AFM SEM and XRD to build reliable feedback loops between theory and measurement.

Experimental Research Magnetic Phase Transitions *2023 to 2026*
Soft Matter and Nanophysics Laboratory University of Dhaka

- Performed temperature and field dependent magnetization measurements on La0.55CaxSr0.45xMnO3 manganites to study dimensionality tuning through chemical substitution.
- Extracted critical exponents using modified Arrott plots and Kouvel Fisher analysis showing evolution of universality class with compositional modification.
- Developed protocols to minimize hysteresis artifacts improving extraction of intrinsic critical behavior in correlated oxides.

Computational Infrastructure Development *2023 to 2026*

- Maintained GPU enabled Linux clusters for VASP calculations and implemented SLURM scheduling workflows ensuring reproducibility for large scale DFT studies.
- Developed convergence testing pipelines for precision control in defect and phonon calculations.

Started PhD in Physics *Aug 2026 to Present*

- Joined as a PhD student at the department of physics, Auburn University, USA

Technical Skills

Electronic Structure: VASP VASPKIT VESTA
Methods: Spin polarized DFT defect formation energies phonon dispersion Bader charge NEB reaction pathways DOS band structure convergence testing
Programming: Python C++ Fortran MATLAB
HPC: MPI parallelization SLURM workflow design
Experimental: Hydrothermal synthesis UV visible spectroscopy magnetization measurements AFM SEM XRD
Analysis: Critical exponent extraction vibrational signature analysis defect state identification
Documentation: LaTeX

Publications and Presentations

Manuscripts in Preparation:

- *Electronic structure modification through defects and curvature in TiO2 based low dimensional systems.*
- *Critical behavior and universality near the ferromagnetic to paramagnetic transition in La0.55CaxSr0.45xMnO3 manganites.*

Conference Presentations:

- Electronic Structure Evolution in TiO2 Nanotubes Research Fair University of Rajshahi 2025.
- Critical Behavior in Doped Manganites Bose Centre Research Fair 2024.
- Structure Dependent Electronic Behavior in Oxide Nanostructures International Conference on Physics Bangladesh Physical Society 2024.

Teaching and Mentoring

Teaching Assistant Experimental Physics *2025 to Feb 2026*
BRAC University Dhaka

- Guided laboratory courses for more than sixty students supervising experiments and evaluating technical reports.

Mentor Computational Condensed Matter Projects *2023 to 2026*

- Trained students in DFT workflows convergence testing defect analysis and reproducible HPC practices.

Awards and Honors

- International Science Programme Fellowship Uppsala University.
- Perfect GPA in all experimental physics courses University of Dhaka.
- Bangladesh Physics Olympiad problem development and evaluation.

Languages

English professional working proficiency · Bengali native

References

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Prof Dr Alamgir Kabir
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