

## **Kapil Adhikari, Ph. D.**

Adjunct Faculty of Physics

Tribhuvan University

Prithvi Narayan Campus, Pokhara, Nepal

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### **Professional Profile**

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Computational material scientist passionate about teaching physics and designing low-cost research projects on physics and material sciences for undergraduate and graduate programs.

### **Education**

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- 2012 **Ph.D.: Computational Condensed Matter Physics**, CGPA: 4.0/4.0  
University of Texas at Arlington – Arlington, TX, USA
- 2007 **Master of Science: Physics** (Solid State Physics), First Division  
Tribhuvan University, Kathmandu, Nepal

### **Experience**

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- 05/2017 – Current **Adjunct Faculty of Physics**  
**Tribhuvan University**  
Prithvi Narayan Campus – Pokhara, Nepal
- 02/2017 – Current **Coordinator**  
**Physics Research Initiatives**  
Pokhara, Nepal
- 10/2016 – Current **Full-Time Faculty of Physics**  
**Tribhuvan University**  
Mt. Annapurna Campus – Pokhara, Nepal
- 10/2015 – 10/2016 **Postdoctoral Research Scientist**  
**Texas A&M University at Qatar** – Doha, Qatar
- Use modern atomistic simulations to investigate the mechanisms governing the radiation damage in materials in general.
  - Assist in the supervision of graduate research assistant or undergraduate students who are working on research related to the project.

- Computational and theoretical studies on corrosion of metal surface.
- Benchmarking of computational chemistry/physics programs in high performance computing environment.
- Provide support and advise to researchers in the use of parallel computational resources.

05/2015 – 09/2015

**Postdoctoral Fellow**

**University of Delaware** – Delaware, NE, USA

- Computational studies on co-crystals of energetic materials.
- Assist with the mentoring of undergraduate and graduate students.

06/2013 – 04/2015

**Postdoctoral Fellow and non-tenure-track instructor**

**Michigan Technological University** – Houghton, MI, USA

- Teach course on Molecular Structures (CH3520) to senior undergraduates.
- Computational studies on molecular crystals.
- Provide assistance in dealing with technical issues related to computing facilities (compilation and benchmarking of computational chemistry programs)
- Assist with the mentoring of undergraduate and graduate students.

09/2012 - 05/2013

**Postdoctoral Fellow**

**The University of Texas at Arlington** – Arlington, TX, USA

Numerical Modeling of actinides in solid state and surface, their electronic structure calculation and their interaction with environment to find a viable way to manage nuclear waste materials.

09/2012-12/2012

**Physics Instructor**

**The College of Health Care Professions**, Dallas, TX, USA

- Prepare weekly lesson plans, lectures and testing materials; instruct class
- Manage classroom to provide optimal learning environment
- Advise students regarding academic progress

08/2008 - 08/2012

**Graduate Teaching/Research Assistant**

**The University of Texas at Arlington** – Arlington, TX, USA

- Modeling of nanostructures and study of their electronic structures.
- Computational studies of actinides and their interactions with environment.
- Conducted lab sessions for undergraduate level physics 1441 and 1443. Instructor for Modern Physics 3183.
- Instructor for General College Physics I and II (1441, 1442) for two semesters.
- Assistant instructor for graduate level quantum mechanics 5307.

12/2005 - 06/2008

### **Lecturer of Physics**

**Kathmandu Institute of Science and Technology, Nepal**

- Worked as a full time lecturer of physics.
- Moderated students' project works, experiments and presentations.
- Formulated students' aptitude test on various topics of natural sciences.

### **Courses Taught on an Independent Basis**

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- **The University of Texas at Arlington, Arlington, TX**
  - General College Physics I (PHYS 1441)
  - General College Physics II (PHYS 1442)
- **The College of Health Care Professions, Dallas, TX**
  - College Physics (PHYS 1401)
- **Michigan Technological University, Houghton, MI**
  - Physical Chemistry II – Molecular Structures (CH3520)

### **Courses Taught as an Assistant/Laboratory Instructor**

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- **The University of Texas at Arlington, Arlington, TX**
  - General College Physics I (PHYS 1441)
  - General College Physics II (PHYS 1442)
  - Modern Physics (PHYS 3183)
  - Quantum Mechanics (PHYS 5307)

### **Areas of Expertise**

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- Expert in using two learning management systems (LMS) ---- Canvas and Blackboard.
- Physics teaching at undergraduate/graduate level.

- Designing low-cost, short-term research projects on physics and material sciences for undergraduate students.
- Well-versed in computer simulation of materials.
- Proficiency in FORTRAN, MPI, MATHEMATICA, MATLAB.
- Proficiency in Gaussian 09, SIESTA, WIEN2k, VASP, CRYSTAL 09, and Quantum Espresso suites of programs for electronic structure calculations.
- Good knowledge in UNIX based high performance computation.
- Theoretical and computational nanoscience.

## Research Interests

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- Low cost physics experiments and simulations for undergraduate programs.
- Theoretical and computational studies on polymorphism in molecular crystals.
- Phase transition in crystalline materials.
- Electronic structure and transport properties of nanotubes, nanocones and nano-clusters.
- Metal-Organic-Frameworks and other nanoporous materials.

## Thesis/Dissertation

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PhD Dissertation: "Silicon Carbide at Nanoscale: Finite Single-Walled to "Infinite" Multi-Walled Tubes"

MS Thesis: "Surface Modification of Polycarbonate by Low Pressure DC Glow Discharge"

## Awards

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- Pruett Postdoctoral Fellowship, Michigan Technological University, Houghton, MI, 2013.
- Graduate Dean's Dissertation Fellowship, University of Texas at Arlington, 2012.
- Graduate Dean's Doctoral Fellowship, University of Texas at Arlington, 2008-2012.
- John D. McNutt Memorial Scholarship, University of Texas at Arlington, 2010.
- STEM Fellowship, University of Texas at Arlington, 2008-2010.

## Publications

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1. Kapil Adhikari, Aurab Chakrabarty, Othmane Bouhali, Normand Mousseau, Charlotte S Becquart, Fedwa El-Mellouhi, "Benchmarking the performance of plane-wave vs. localized orbital basis set methods in DFT modeling of metal surface: a case study for Fe-(110) " Journal of Computational Science 29, 163 –

167 (2018)

DOI: <https://doi.org/10.1016/j.jocs.2018.10.008>

2. K. Adhikari, K. M. Flurchick, L. Valenzano, "Effects of Volumetric Expansion in Molecular Crystals: A Quantum Mechanical Investigation on Aspirin and Paracetamol Most Stable Polymorphs", *Chemical Physics Letters* 621, 109-116 (2015)  
DOI: <https://doi.org/10.1016/j.cplett.2014.12.059>
3. K. Adhikari, K. M. Flurchick, L. Valenzano, "Volumetric influence on the mechanical behavior of organic solids: the case of aspirin and paracetamol addressed via dispersion corrected DFT", *Chemical Physics Letters* 630, 44-50 (2015)  
DOI: <https://doi.org/10.1016/j.cplett.2015.04.024>
4. K. Adhikari, K. M. Flurchick, L. Valenzano, "A Hybrid Density Functional Study on the Effects of Pressure on Paracetamol and Aspirin Polymorphs", *Computational and Theoretical Chemistry* 1062, 90-98 (2015)  
DOI: <https://doi.org/10.1016/j.comptc.2015.03.020>
5. K. Adhikari, A. K. Ray, "Magnetic silicon carbide nanotubes by 3d transition metal atom functionalization" *Physics Letters A* 377 2147-2153 (2013).  
DOI: <https://doi.org/10.1016/j.physleta.2013.06.005>
6. K. Adhikari, M. N. Huda, A. K. Ray, "Anomalous Dependence of Band Gaps of Binary Nanotubes on Diameters", *Journal of Computational and Theoretical Nanoscience* 8, 1502-1508 (2011).  
DOI: <https://doi.org/10.1166/jctn.2011.1842>
7. K. Adhikari, A. K. Ray, "Cluster Modeling of Three Types of Armchair Silicon Carbide Nanotubes", *European Physical Journal D* 64, 353-363 (2011).  
DOI: 10.1140/epjd/e2011-20280-3
8. K. Adhikari, A. K. Ray, "On the Existence and Stability of Double-Walled Armchair Silicon Carbide Nanotubes", *Solid State Communications* 151, 430-435 (2011).  
DOI: <https://doi.org/10.1016/j.ssc.2011.01.004>
9. K. Adhikari, A. K. Ray, "Carbon- and Silicon-Capped Silicon Carbide

- Nanotubes: An Ab Initio Study", *Physics Letters A* 375, 1817-1823 (2011).  
DOI: <https://doi.org/10.1016/j.physleta.2011.03.016>
10. K. Adhikari, A. K. Ray, "Stabilities of Silicon Carbide Nanocones: A Nanocluster Based Study", *Journal of Nanoparticle Research* 14, 1-14 (2012).  
DOI: 10.1007/s11051-012-0816-6
  11. Arvydas Tamulis, Kristina Majauskaite, Visvaldas Kairys, Krzysztof Zborowski, Kapil Adhikari, Sarunas Krisciukaitis, "Spintronic characteristics of self-assembled neurotransmitter acetylcholine molecular complexes enable quantum information procession in neural network and brain", *Chemical Physics Letters* 660, 189-198 (2016).  
DOI: <http://dx.doi.org/10.1016/j.cplett.2016.08.017>
  12. Jingtuo Zhang, Mu Yang, Wafa Mazi, Kapil Adhikari, Mingxi Fang, Fei Xie, Loredana Valenzano, Ashutosh Tiwari, Fen-Tair Luo, Haiying Liu, "Unusual Fluorescent Responses of Morpholine-Functionalized Fluorescent Probes to pH via Manipulation of BODIPY's HOMO and LUMO Energy Orbitals for Intracellular pH Detection", *ACS Sensors* 1, 158-165 (2015)  
DOI: 10.1021/acssensors.5b00065
  13. H. Chen, K. Adhikari, A. K. Ray, "An Ab Initio Study of Atomic Hydrogen and Oxygen Adsorptions on Armchair Silicon Nanotubes" *Journal of Computational and Theoretical Nanoscience* 9, 495-504 (2012).  
DOI: 10.1166/jctn.2012.2051
  14. K. Adhikari, A. K. Ray, "An ab-initio study on the convergence of electronic properties of SiC nanotubes", *Himalayan Physics* 3, 69-73 (2012).  
DOI: <http://dx.doi.org/10.3126/hj.v3i0.7309>
  15. D. P. Subedi, D. K. Madhup, K. Adhikari, U. M. Joshi, "Low Pressure Plasma Treatment for the Enhancement of Wettability of Polycarbonate", *Indian Journal of Pure and Applied Physics* 46, 540-544 (2008).  
DOI: <http://nopr.niscair.res.in/handle/123456789/1904>
  16. K. Adhikari, D. K. Madhup, B. Niraula, and D. P. Subedi "Surface Treatment of Polycarbonate on Low Pressure DC Glow Discharge", *Annual Proceeding of Nepal Physical Society, Kathmandu, Nepal* 22, 8 (Special Issue) (2006).
  17. K. Adhikari, D. K. Madhup, R. Khanal, and D. P. Subedi, "Etching of

Polycarbonate by Low Pressure DC Glow Discharge", *Annual Proceeding of Nepal Physical Society*, Kathmandu, Nepal 22, 6 (Special Issue) (2006)

## Reference Materials

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1. K. Adhikari, A. K. Ray, "Silicon Carbide Nanotubes: from Finite Single-Walled to Infinite Multi-Walled", *Journal of Computational and Theoretical Nanoscience* 9, 1801-1829, (2012). (Invited **Review Article**, Published on the Special Issue)

## Research Reports

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1. Surface Energetics of Paracetamol: A Theoretical Study, **2014**, Michigan Technological University, Houghton, MI 49931, USA
2. Benchmarking the Performance of Planewave vs. Localized Orbital Basis Set in DFT Modeling of Metal Surface, **2016**, Texas A&M University at Qatar, Education City, Qatar
3. Computational Study of Electronic and Optical Properties of p-group Atomic Adsorption on alpha-Al<sub>2</sub>O<sub>3</sub> (0001), **2016**, Texas A&M University at Qatar, Education City, Qatar

## Research Papers Presented at Conferences

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1. Loredana Valenzano, Kapil Adhikari, "Energetics of Active Pharmaceutical Ingredients (APIs) Surfaces: A Quantum Chemical Study, poster presented at Gordon Research Conference on Crystal Engineering, Waterville Valley, NH, June 1-6, 2014
2. D. T. Beegle, K. Adhikari, L. Valenzano, "Assembling the peptidoglycan bacterial cell wall: A stepwise quantum chemical approach", paper presented at the 247<sup>th</sup> American Chemical Society National Meeting & Exposition, Dallas, TX, March 16-20, 2014.
3. K. Adhikari, K. M. Flurchick, L. Valenzano, "Mimicking thermal effects on bulk properties of molecular crystal polymorphs and cleaving their surfaces from first principles", paper presented at the 247<sup>th</sup> American Chemical Society National Meeting & Exposition, Dallas, TX, March 16-20, 2014.
4. K. Adhikari, A. K. Ray, "An Ab Initio Study of the Interaction between 3d Transition Metal Atoms and Silicon Carbide Nanotubes", paper presented at the March, 2013 Meeting of the American Physical Society, Bulletin of the

American Physical Society, 58, 2013.

5. K. Adhikari, M. N. Huda, A. K. Ray, "Anomalous dependence of band gaps of binary nanotubes on diameters", poster presented at the March, 2012 Meeting of the American Physical Society, *Bulletin of the American Physical Society*, 57, p. 503.
6. K. Adhikari, A. K. Ray, "A Nanocluster Based Study of Silicon Carbide Nanocones: Existence and Stability", paper presented at the March, 2012 Meeting of the American Physical Society, *Bulletin of the American Physical Society*, 57, p. 459.
7. K. Adhikari, A. K. Ray, "A Hybrid Density Functional Study of Capped Silicon Carbide Nanotubes", paper presented at the March, 2011 Meeting of the American Physical Society, *Bulletin of the American Physical Society*, 56, p.269.
8. K. Adhikari, A. K. Ray, "An *Ab Initio* Study of SiC Double-Walled Nanotubes of Types 2 and 3", poster presented at the March, 2011 Meeting of the American Physical Society, *Bulletin of the American Physical Society*, 56, p.420.
9. H. Chen, K. Adhikari, A. K. Ray, "An *Ab Initio* Study of Atomic Hydrogen and Oxygen Adsorptions on Armchair Si Nanotubes", poster presented at the March, 2011 Meeting of the American Physical Society, *Bulletin of the American Physical Society*, 56, p. 420.
10. K. Adhikari, A. K. Ray, "A Hybrid Density Functional Study of Double-Walled Armchair SiC Nanotubes", paper presented at the March, 2010 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR10>, *Bulletin of the American Physical Society*, 55, p 350.

### **Seminars and Invited Presentation**

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"Silicon Carbide Nanostructures: From Tubes to Cones",  
Department of Chemistry, Michigan Technological University (09/27/2013)

### **Referee Service**

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- International Journal of Hydrogen Energy
- Chemical Physics Letters
- Physical Chemistry Chemical Physics
- Nanoscale
- RSC Advances



- Journal of Materials Chemistry B
- Modern Physics Letters B
- International Journal of Modern Physics B
- Surface Review and Letters

## **Affiliations**

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- Member of American Physical Society
- Member of American Chemical Society
- Member of Phi Kappa Phi