CURRICULUM VITAE

Personal :

Name : Narayan Prasad Adhikari
Date of Birth: March 10, 1969
Marital Status: Married

Present Address : Central Departmentof Physics,
Tribhuvan University, Kirtipur,
Kathmandu, Nepal

Home Address: Kirtipur Municipality -3, Kirtipur,
Kathmandu
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WEB: https://scholar.google.com/citations?user=VhEXmuEAAAAJ&hl=en

Education:

Ph. D., 2001 Physics from Martin-Luther University, Halle/Saale, Germany Thesis title: " *Interfacial properties and phase behavior of unsymmetric polymer blends*" Supervisor: **Prof. Ekkehard Straube**

Diploma, 1998 Condensed Matter Physics from The Abdus Salam International Center for Theoretical Physics, Trieste, Italy,
GPA: 3.09 (Max. 4.0) Thesis title: " *Calculations of the energy in two weakly coupled Bose- Einstein Condensates*"
Supervisor: **Prof. Stefano Fantoni**

M. Sc. 1996 Physics From Tribhuvan University, Kirtipur, Kathmandu, Nepal with Distinction (75.3%) ranked **First**
Thesis title: " *Size effects in metal clusters*"
Supervisor: **Prof. Devendra Raj Mishra**

B. Sc. 1993 Physics/Math/Statistics From Amrit Campus, Kathmandu with Distinction (78.1%) ranked **Second**
(Tribhuvan University, Kathmandu, Nepal)

Post Doctoral Experiences:

1. October 2001 – August 2002: Rice University, H ouston, Texas, USA.
   Supervisor: **Prof. Jacqueline Goveas**
2. September 2002 – May 2004: Rensselaer Polytech nic Institute, Troy, New York,
   Supervisor: **Prof. Sanat Kumar**
3. October 2004 – December 2005: Max-Planck Insti tute for Polymer Research, Mainz, Germany, Supervisor: **Prof. Kurt Kremer**

Research Interest:

The understanding of the structural and dynamical properties of macromolecular systems is a central objective of my research work. To achieve complex self-assemblies and functional materials, the understanding of basic structural and dynamical, or relaxational aspects and mechanisms is an indispensable part of rational materials design. The theory of single macromolecular chain is already developed and well known. However there are many unsolved problems by this theory in this area. It

demands either computer modeling or experimental study of such a complex but very interesting problem. I use systematic multiscale modeling strategies to study such complicated amorphous and structurally organized macromolecular systems. My research in this area is especially focused on the understanding of biomoleculaes using multi scale techniques.

I am also interested to study the electronic structure of solids using the first-principles calculations. I have been working on the electronic, vibrational and magnetic properties of disordered binary and ternary alloys. Further I have been studying the phase stability and phase diagrams of alloy systems. I work to develop the Density Functional theory for excited states in disordered solids. In this area my research interest is to study the phase diagram of clathrate systems like mthane-clathrate in the very high pressure. Other useful systems in this regard include environmentally significant systems like ozone clusters, water clusters and fundamentally as well as technologically important systems like Graphene, Graphene/other monolayer hetero structure systems.

Collaborations (Only those institutes/Universities are mentioned in which M.Sc. or Ph.D. students of Central Department of Physics, TU have visited or visiting near future).

1. Prof. Somen Bhattacharjee, Institute of Physics, Bhuvaneshwar, India
2. Prof. Shobhana Narasimhan, JNCASR, Bangalore, india
3. Prof. Sandro Scandolo, ICTP, Trieste, Italy
4. Prof. Biplab Sanyal, Uppsala University, Sweden
5. Prof. Ravi Pandey, Michigan Tech university, USA
6. Prof. Prem Chapagain & Prof. Bernard Gerstman, Florida International University, USA.
7. Prof. Arghya Taraphder, Indian Institute of Technology Kharagpur, India
8. Prof. Hassanali Ali, ICTP, Trieste, Italy

Working Experiences:

1. Worked as an Assistant Professor from July 1997 to July 2009 at the Central Department of Physics, Tribhuvan University (CDPTU), Kirtipur, Kathmandu, Nepal
2. Working as an Associate Professor from July 2009 to 2013 at (CDPTU).
3. Working as a Professor the Central Department of Physics, Tribhuvan University (CDPTU), Kirtipur, Kathmandu, Nepal
   I was in study leave from October 1998 to September 2005.

Computer Skills:

1. **Operating systems**: Unix, Linux and Windows
2. **Languages**: Fortran, C and C++
3. **Supercomputing**: Experience of Cray T/3E computing facilities of Max-Planck Society, Germany.
4. **Windows and Linux:** Networking and security

Supervision of Ph.D. Thesis (Tribhuvan University)

1. **Gopi Chandra Kaphle** (2010 – 2014) in joint supervision with Prof. Abhijit Mookerjee (SN Bose Center, Kolkata)
2. **Nurapati Pantha** (2011 – 2017) in joint supervision with Prof. Sandro Scandolo (ICTP)
3. **Saran Lamichhane** (2013 – 2019)
4. **Sunil Pokharel** (2014 – 2019)
5. Rajendra Koirala (2017 – ongoing)
6. Shyam Prakash Khanal (2017-ongoing)
7. Hari K Neupane (2019 – ongoing)
8. Ms. Bidhya Thapa (2020 – ongoing)
9. Jhulan Powrel (2019 – ongoing)

Supervision of M. Sc. Thesis (Tribhuvan University)

I have supervised More than 100 M.Sc students at Tribhuvan University for their work of Dissertation/Project.

Serving as a Research Committee Member of Institute of Science and Technology, Tribhuvan University (2016 Jan – till date)

Serving as a Research Committee Member at Central Department of Physics (Since 2008 - till date)

Serving as a Subject Committee Member of physics at Tribhuvan University (Since 2014 - till date)

Professional Society/Research Center:

1. **Life member;** Nepal physical society
2. **Member;** American institute of chemical engineers (AICHE) (2002-2004)
3. **Member:** Institute of Electrical and Electronics Engineers (IEEE) (2008- till date)
4. **Associate Member (January 2009-December 2015):** the Abdus Salam International Center for Theoretical Physics, Trieste, Italy.

Organization:

1. **Editor;** Nepal physical society (2007-2009)
2. **Deputy coordinator**; Nepal Physics Olympiad Committee (2006 – 2008)
3. **Member**; Organizing committee; Kathmandu Autumn School on Physics of New Materials, 2007, Kathmandu.
4. **Coordinator**; Nepal Physics Olympiad Committee (2008 – 2009)
5. **Member**; Organizing Committee (2007); symposium on plasma physics and material science, Kathmandu, Nepal
6. **Member**; Organizing committee (2008); symposium on plasma physics and material science, Kathmandu, Nepal
7. **Secretary**; International Conference on Frontiers of Physics 2009 (ICFP 2009); Kathmandu, Nepal
8. **Leader**; Nepal Physics Olympiad team in 38th International Physics Olympiad, 2007, Isfahan, Iran.
9. **Leader**; Nepal Physics Olympiad team in 40th International Physics Olympiad, 2007, Merida, Mexico
10. **Member;** Organizing committee (October 12-14, 2011); International Symposium on Lightning Protection; Kathamndu, Nepal
11. **Member**; Organizing committee, Polychar 19, (March20-24), Kathmandu,
12. **Member**; Organizing committee, Kathmandu Symposium on Advanced Materials, (May 9-12, 2012), Kathmandu, Nepal
13. **Coordinator**: Kathmandu summer School on *ab initio* simulation of solids, April 14-20, 2013
14. **Coordinator:** National workshop in computational physics, April 27-May 2, 2014
15. **Secretary:** Nepal Physical Society (Since January 2016 – till date)

Publications:

NOTE: This list does not include my publications in abstract books of various conferences (~25 Abstracts) and books/journals I edited when I served as Editor of Nepal Physical society.

Published papers in International Peer Reviewed Journals

1. Effect of temperature on transport properties of cysteine in water; R P Koirala, HP Bhusal, SP Khanal, NP Adhikari; AIP Advances 10 (2), 025122 (2020)
2. Transport properties of zwitterion glycine, diglycine, and triglycine in water ; SP Khanal, YP Kandel, NP Adhikari; AIP Advances 9 (6), 065303 (2019)
3. Transport properties of methane, ethane, propane, and n-butane in water
   S Pokharel, N Aryal, BR Niraula, A Subedi, NP Adhikari
   Journal of Physics Communications; 2 (6), 065003(2018)
4. Molecular dynamics study of diffusion of xenon in water at different temperatures
   NK Nepal, NP Adhikari
   Scientia Bruneiana, Vol. 16, 12-21(2018)
5. Basis Set Effect on Alkaline-Earth Fluoride Structures
   S Lamichhane, NP Adhikari
   Journal of Computational and Theoretical Nanoscience 14 (5), 2315-2318(2017)
6. Study of structural and transport properties of argon, krypton, and their binary mixtures at different temperatures
   S Ghimire, NP Adhikari
   Journal of molecular modeling 23 (3), 94 (2017)
7. Diffusion coefficients of nitric oxide in water: A molecular dynamics study
   S Pokharel, N Pantha, NP Adhikari
   International Journal of Modern Physics B 30 (27), 1650205 (2016)
8. First-Principles Study of Adsorption of Halogen Molecules on Graphene-MoS2 Bilayer Hetero-system
   S Lamichhane, P Lage, GB Khatri, N Pantha, NP Adhikari, B Sanyal
   Journal of Physics: Conference Series 765 (1), 012011 (2016)
9. Electronic Structures and Magnetic Properties of NiAl and Ni3Al
   S Lamichhane, GC Kaphle, NP Adhikari
   Quantum Matter 5 (3), 356-361 (2016)
10. First-Principles Study of Oxygen Clusters (O) n, n= 2–9 and Ozone
    NP Adhikari
    Quantum Matter 5 (3), 379-382 (2016)
11. Adsorption and Dissociation of Nitrogen and Hydrogen Molecules on Platinum (Pt) Clusters
    GC Kaphle, NP Adhikari, A Mookerjee
    Quantum Matter 5 (3), 348-355 (2016)
12. Mixing behaviour of Ni–Al melt at 1873 K
    SK Yadav, S Lamichhane, LN Jha, NP Adhikari, D Adhikari
    Physics and Chemistry of Liquids 54 (3), 370-383 (2016)
13. Molecular dynamics study of diffusion of krypton in water at different temperatures
    D Bhandari, NP Adhikari
    International Journal of Modern Physics B 30 (11), 1650064 (2016)
14. Study of Spin Glass Behavior in Disordered Pt x Mn1− x Alloys: An Augmented Space Recursion Approach

GC Kaphle, N Adhikari, A Mookerjee
Advanced Science Letters 21 (9), 2681-2687 (2015)

15. Hydrogen storage on palladium adsorbed graphene: A density functional theory study
N Pantha, A Khaniya, NP Adhikari
International Journal of Modern Physics B 29 (20), 1550143 (2015)
16. Decomposition of methane hydrates at high pressure: a density-fuctional theory study
N Pantha, NP Adhikari, S Scandolo
High Pressure Research 35 (3), 231-238 (2015)
17. First-principles study of the interaction of hydrogen molecular on Na-adsorbed graphene
N Pantha, K Belbase, NP Adhikari
Applied Nanoscience 5 (4), 393-402 (2015)
18. First-principles study of the stability of graphene and adsorption of halogen atoms (F, Cl and Br) on hydrogen passivated graphene
DB Karki, NP Adhikari
International Journal of Modern Physics B 28 (21), 1450141 (2014)
19. Temperature dependence of diffusion coefficient of nitrogen gas in water: A molecular dynamics study
K Sharma, NP Adhikari
International Journal of Modern Physics B 28 (14), 1450084 (2014)
20. Temperature dependence of diffusion coefficient of carbon monoxide in water: A molecular dynamics study
I Poudyal, NP Adhikari
Journal of Molecular Liquids 194, 77-84 (2014)
21. Band gap tunning in BN-doped graphene systems with high carrier mobility
Kaloni TP, Joshi RP, Adhikari NP, Schwingenschlögl
Applied Physics Letters 104, 073116 (2014)
22. A molecular dynamics study of oxygen gas in water at different temperatures
SK Thapa, NP Adhikari
International Journal of Modern Physics B 27 (08), 1350023 (2013)
23. First-Principles study of adsorption of alkali metals (Li, Na, K) on graphene
BD Oli, C Bhattarai, B Nepal, NP Adhikari
Advanced Nanomaterials and Nanotechnology, 515-529 (2013)
24. A study of magnetism in disordered Pt–Mn, Pd–Mn and Ni–Mn alloys: an augmented space recursion approach
GC Kaphle, S Ganguly, R Banerjee, R Banerjee, R Khanal, CM Adhikari, NP Adhikari & A Mookerjeee
Journal of Physics: Condensed Matter 24 (29), 295501 (2012)
25. Interfacial Tension and Width of an Asymmetric Polymer Mixture
NP Adhikari
Macromolecular Symposia 315 (1), 15-23 (2012)
26. Molecular dynamics study of diffusion of heavy water in normal water at different temperatures
U Dahal, NP Adhikari
Journal of Molecular Liquids 167, 34-39 (2012)
27. Molecular Dynamics Study of Diffusion of Different Inert Gases Like Neon and Argon in Water at Different Temperatures
HB Moktan, A Panday, NP Adhikari

International Journal of Modern Physics B 26 (03), 1250016 (2012)

28. Phase separation in mixtures of flexible and semiflexible polymers
    NP Adhikari, E Straube
    Polymer journal 43 (9), 751 (2011)
29. Theoretical and experimental study of hydrogen bonded liquids with water as an example
    NP Adhikari, H Paudyal, A Tiwari, M Johri
    Journal of molecular liquids 158 (2), 80-91 (2011)
30. Dielectric Behavior Of Binary Solutions Of Thermacol In Organic Solvents
    NP Adhikari, P Bhattarai, MM Aryal, DR Mishra
    Journal of Bangladesh Academy of Sciences 35 (2), 211-220 (2011)
31. MM Aryal, DR Mishra, D Paudyal, S Byahut, NB Maharjan, NP Adhikari, TP Das
    HFI/NQI 2007, 51-57 (2008)
32. Ethylbenzene diffusion in polystyrene: United atom atomistic/coarse grained simulations and experiments
    VA Harmandaris, NP Adhikari, NFA van der Vegt, K Kremer, BA Mann
    Macromolecules 40 (19), 7026-7035 (2007)
33. Multiscale modeling of the synthesis of quantum nanodots and their arrays
    N Adhikari, X Peng, A Alizadeh, S Nayak, SK Kumar
    Theoretical and Computational Chemistry 18, 85-99 (2007)
34. Hierarchical modeling of polystyrene: From atomistic to coarse-grained simulations
    VA Harmandaris, NP Adhikari, NFA van der Vegt, K Kremer
    Macromolecules 39 (19), 6708-6719 (2006)
35. Multiscale modeling of the surfactant mediated synthesis and supramolecular assembly of cobalt nanodots
    NP Adhikari, X Peng, A Alizadeh, S Ganti, SK Nayak, SK Kumar
    Physical review letters 93 (18), 188301 (2004)
36. Effects of slip on the viscosity of polymer melts
    NP Adhikari, JL Goveas
    Journal of Polymer Science Part B: Polymer Physics 42 (10), 1888-1904 (2004)
37. Interfacial properties of asymmetric polymer mixtures
    NP Adhikari, E Straube
    Macromolecular theory and simulations 12 (7), 499-507 (2003)
38. Interfacial properties of flexible and semiflexible polymers
    NP Adhikari, R Auhl, E Straube
    Macromolecular theory and simulations 11 (3), 315-325 (2002)
39. Interfacial properties of the mixture of flexible and semiflexible polymers
    NP Adhikari, E Straube
    AIP Conference Proceedings 574 (1), 252-253 (2001)

Preprints

1. Transport properties of Valine in water at different temperatures
    D Pandey, NP Adhikari
    arXiv preprint arXiv:1809.04996

2. Molecular Dynamics Study of Transport Properties of Cysteine in Water
    H Prasad Bhusal, N Prasad Adhikari
    arXiv preprint arXiv:1809.08768

3. Transport properties of Gamma-Aminobutyric Acid in water
   E Mishra, NP Adhikari
   arXiv preprint arXiv:1806.09956

4. Diffusion of Zwitterion Glycine, Diglycine, and Triglycine in Water
   YP Kandel, NP Adhikari
   arXiv preprint arXiv:1706.05491 (2017)
5. First-principles DFT study for the structural stability of Hydrogen passivated graphene (H-graphene) and atomic adsorption of oxygen on H-graphene
   DB Karki, NP Adhikari
   arXiv preprint arXiv:1404.6446 (2014)
6. Dielectric Relaxation of Water: Theory and Experiment
   NP Adhikari, H Paudyal, M Johri
   Abdus Salam International Centre for Theoretical Physics(Priprint) (2010)

Publications in National Refereed Journals

1. First-principles Study of Electronic and Magnetic Properties of Manganese Decorated Graphene
   BP Paudel, N Pantha, NP Adhikari
   Journal of Nepal Physical Society 3 (1), 24-34 (2016)
2. Structural and electronic properties of perovskite hydrides ACaH3 (A= Cs and Rb)
   S Lamichhane, B Aryal, GC Kaphle, NP Adhikari
   BIBECHANA 13, 94-99 (2015)
3. First-principles study of a molecular adsorption of fluorine on monolayer MoS2
   H Paudyal, N Pantha, NP Adhikari
   BIBECHANA 13, 50-59 (2015)
4. Structure and Symmetrization of Hydrogen Bonding in Ices VIII and X at High Pressure: A Density Functional Theory Approach
   N Pantha, NP Adhikari
   Journal of Institute of Science and Technology 19 (2), 14-18(2015)
5. Study of Electronic and Magnetic Properties of CuPd, CuPt, Cu 3 Pd and Cu 3 Pt: Tight Binding Linear Muffin-Tin Orbitals Approach
   S Dahal, G Kafle, GC Kaphle, NP Adhikari
   Journal of Institute of Science and Technology 19 (1), 137-144 (2015)
6. Hydrogen storage on platinum decorated graphene: a first-principles study
   S Lamichhane, N Pantha, NP Adhikari
   Bibechana 11, 113-122 (2014)
7. Electronic structure and magnetic properties of bulk elements (Fe and Pd) and ordered binary alloys (FePd and Fe3Pd): TB-LMTO-ASA
   S Pandey, GC Kaphle, NP Adhikari
   BIBECHANA 11, 60-69 (2014)
8. First-principles study of solid methane at high pressure
   N Pantha, J Acharya, NP Adhikari
   BIBECHANA 12, 70-79 (2014)
9. **.** Multi-scale Modeling in Computational Material Science
   N. P. Adhikari,
   Proceedings of Nepal Physical society, 22, 30(2006).
10. Electronic structure in metal clusters
    N.P. Adhikari and D.R. Mishra,

Journal of Nepal Physical Society, 15,13(1998).

11. Thickness dependence of Fermi wave vector in thin bismuth films
N.P. Adhikari and D.R. Mishra,
Journal of Nepal Physical Society, 13, 23(1996).

Medals and Awards:

1. " **Amrit Medal 1993**", for securing highest marks among the students of Amrit Campus, in final exams of Tribhuvan University in B. Sc. level
2. " **Chhatra Prasad Mainali Gold Medal 1996**", for securing highest marks among the students of M.Sc. in Physics, Tribhuvan University. Awarded by the King Birendra Bir Bikram Shah Dev.
3. " **Mahendra Bidhya Bhushan "B"** ", awarded by the King Birendra Bir Bikram Shah Dev in 1997.
4. " **TWAS Award in Physics 2007**", awarded by Third world academy of sciences, Trieste, Italy for the contributions in nanoscience, polymer science and computational physics.

Research Projects/Grants: (I have mentioned only those in which I am Principal Investigator)

1. **The World Academy of Sciences**: *ab initio molecular dynamics study of phase diagram of methane (2013-2014)*. The grants is for $15,000.00 and it has been used to establish uninterrupted power solar power system and a 20 processors supercomputer at Central department of Physics, Tribhuvan University
2. **American Physical Society**, Travel Grants for 2011-2012 to carry on joint research with Dr. Prem Chapagain (Florida International University, FL, USA) " *Quantum Mechanical/Molecular Mechanics study of mCherry*"
3. **Nepal Academy of Science and Technology (NAST)** has funded a research project to carry on research on " *First-Principles Study of Some Simple Systems of Biological Significance*" in the Central Department of Physics, Tribhuvan University, Kirtipur, 2009; Total amount (NRS 60,000.00).
4. **NET-56, Grants from ICTP/TWAS** *for the first-principles calculations projects to be conducted at CDPTU*. It included fellowship for students from CDPTU
5. **Nepal Academy of Science and Technology (NAST)** has funded a research project to carry on research on " *First-Principles Study of Some Environmentally Significance System like Methane Clathrate*" in the Central Department of Physics, Tribhuvan University, Kirtipur, 2009; Total amount (NRS 60,000.00).
8. **University Grants Commission**, Nepal has funded a research project to " *Study the spin glass sytems like PtMn, PdMn, AuFe and CuMn*" in the Central Department of Physics, Tribhuvan University, Kirtipur, 2011; Total amount (NRS 200,000.00).

National and International Conferences:

I have participated and contributed research papers in more than 60 International/National Conferences.

Invited talks (Colloquim)

I have delivered Invited talks in the topics of my research at various universities in USa, Europe, India, Bangladesh and Nepal.

Scholarships:

1. Intelligent scholarship was obtained during the study at high school and at University in I.Sc., B.Sc. and M. Sc. level.

2. ICTP diploma scholarship to study “Condensed M atter Physics” a postgraduate diploma program.

To carry on the further study and perform research in Physics I obtained fellowship for Ph. D. and post doc positions mentioned above.