BIODATA

Personal Data

Name	:-	Dr. Bipul Rakshit
Father's Name	:-	Biswanath Rakshit
Age	:-	34
Sex	:-	Male
Date of birth	:-	08th January 1982
Marital status	:-	Single
Nationality	:-	Indian
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Educational Qualification

- PhD in Physics (2004-2009)
  Theoretical condense matter physics,
  Barkatullah University of Bhopal, MP, India
  (Awarded on 14th April 2009)

Thesis Title: **Phonon Dynamics and Ab-initio Calculations of some Rare-Earth Compounds**
Supervisor: **Dr. Sankar P Sanyal**

- Master of Science (Pure Physics, 2002-2004)
  Specialization in Nuclear Physics.
  Pass with first class distinction with 70.05%
  Maharaja Syajirao University, Baroda, Gujarat, India

- Bachlor of Science (1999-2002)
  Physics (Principle subject)
  & Chemistry & Mathematics (Subsidiary Subjects)
  Pass with first class with 64.58%.
  Maharaja Syajirao University, Baroda, Gujarat, India.

Main area of work

Electronic, magnetic, structural, and mechanical properties of systems at bulk as well as monolayer limit. Electronic structure of Group IV, group III-V as well as group II-VI and there electronic structure variation with thickness.

Charge, orbital and magnetic ordering in p and d band systems, usually perovskites and double perovskites systems. I have expertise and mainly work in density functional theory based codes, **VASP, Quantum-espresso, Siesta and Wien-2k.**

Computer Skills

Operating System: Windows, Linux
Programming: Fortran 77-90 and Shell Programming

Conferences Attended

1. ICONSAT 2014, Punjab Mohali.
2. 52nd Solid State Physics Symposium sponsored by BRNS & DAE, in Mysore Karnataka, during December 27-31, 2007. Participate to present a poster on the topic **"Electronic and Elastic Properties of Rock-Salt LaSb from Density "**
3. 51st Solid State Physics Symposium sponsored by BRNS & DAE, in Bhopal, Barkatullah University during December 26-31, 2006. Participate to present a poster on the topic "**Fluorite structure of Platinum Nitride**"
4. International workshop on **Porting Scientific Application on Computational GRIDs**, by ICTP Trieste, Italy. February 2006
5. 50th DAE Solid State Physics Symposium sponsored by BRNS & DAE, in Bombay BARC, during December 5-9, 2005. Participate to present a poster on the topic "**Experimental and Theoretical Study of III-V Group Semiconductor- GaSb"**

Fellowships (India and Abroad)

Post held	Period of Fellowship		Institute/ University	Name of the funding agency
	From (DD/MM/YY)	To (DD/MM/YY)		
Post-Doc	1st December 2014	Till date	Institute of Physics (IOP)	IOP
Post-Doc	5th August 2012	5th August 2014	SN Bose National Center for Basic Sciences	DST-Nanomission
Post-Doc	4th August 2009	4th August 2012	SN Bose National Center for Basic Sciences	DST
Visiting Fellow	28th May 08	3th July 08	ICTP, Trieste, Italy	ICTP
Senior Research Fellow	19th February 07	18th February 08	Barkatullah University, Bhopal	DAE-BRNS, Mumbai
Visiting Fellow	13th January 07	14th April 07	ENEA, Italy	ENEA, Rome, Italy
Visiting Fellow	4th June 07	7th November 07	ENEA, Italy	ENEA, Rome, Italy
Junior Research	18th February 05	18th February 07	Barkatullah University, Bhopal	DAE-BRNS, Mumbai

Fellow				

Research interest and work Summary

My research interest is in graphene and graphene analogue systems. We start by examining the issue of rippling in graphene[1] grown on a substrate. Several experimental observe rippling in various substrate till C. H. Lui et al.[2] pointed out that ultraflat graphene was possible. Theoretically we have shown that graphene when subjected to biaxial tensile strain can be ripple free. This arises from the linear component proportional to strain that gets added on to the phonon dispersion of the out of plane acoustic branch.

Motivated with earlier theoretical study, that all ionic semiconductors which otherwise favour the wurtzite struct. in the bulk limit, have a graphitic analogue to the one to few monolayers (ML) limit prompted us to study the structural properties and electronic structure of ZnO[3]. We studied the metastable phase of ZnO which is having graphitic like structure, but with lesser out of plane bond length compared to Graphite and BN. The usual GGA/LDA level cal. with the well-known self-interaction error in density functional theory, which result in incorrect position of Zn *d*-states in the valence. This results in a significantly enhanced Zn d character in the valence band, resulting in a mixed nature for the bonding. As the Zn d-states do not benefit in the bonding in a sp^2 geometry, the structure becomes unstable.

We also shows indirect to direct band gap transition when going from bulk to ML in case of ZnO[4]. So the modifications in the electronic structure as a function of thickness and the implications of tuning the band gap will be studied for different semiconductors.

Similarly the thickness dependent band gap tuning, is used to study the ML of transition metal dichalcogenides (Mo-S_2/Se_2, WS_2/Se_2) and BN. A microscopic model is also used to understand the strain driven mechanism in band gap transition[5].

Presently my main focus, is to study the surface properties of the nano-structures (ZnO[6]) and Silicon (001), (5 5 12) surfaces and the change in the work-functions of these layers when capped with gold or silver to provide a theoretical support for these experiments.

1. B. R et al. *PRB* **82**, 153407 (2010).
2. C. H. Lui et al., *Nature (London)*, **462**, 339 (2009).
3. B. R et al. *PRL*., **107**, 085508 (2011).
4. B. R et al. *APL*, ***102***, 143116 (2013)
5. R. Das et al., *PRB* **89**, 115201 (2014).
6. A. Ghosh et al., *Nanotec.* **27**, 125701 (2016).

List of Publications

Paper Published in International Journals

1. **Tuning the work function of randomly oriented ZnO nanostructures by capping with faceted Au nanostructure and oxygen defects: enhanced field emission experiments and DFT studies**
   Arnab Ghosh, Puspendu Guha, Ranjit Thapa, Sinthika Selvaraj, Mohit Kumar, **Bipul Rakshit**, Tapan Dash, Rajshekhar Bar, Samit K Rayand and Parlapalli Venkata Satyam, *Nanotechnology* **27**, 125701 (2016).
   Impact factor: 3.82

2. **Microscopic model for the strain driven direct to indirect bandgap transition in monolayer MoS_2 and ZnO.**
   Ruma Das, **Bipul Rakshit**, Saikat Debnath and Priya Mahadevan, *Phys. Rev. B.* **89**, 115201 (2014)
   Impact factor: 3.767

3. **Indirect to direct band gap transition under uniaxial strain in layered ZnO**
   Bipul Rakshit and Priya Mahadevan, *Applied Phys. Lett.* **102**, 143116 (2013).
   Impact factor: 3.794

4. **Stability of the Bulk Phase of Layered ZnO**
   Bipul Rakshit and Priya Mahadevan, *Phys. Rev. Lett.* **107**, 085508 (2011).
   Impact factor: 7.943

5. **Absence of rippling in graphene under biaxial tensile strain**
   Bipul Rakshit and Priya Mahadevan, *Phys. Rev. B* **82**, 153407 (2010)
   Impact factor: 3.767

6. **Ab initio study of structural, electronic, elastic, and phonon properties of ScN and ScP at ambient and high pressure**
   Premlata Pandit, **Bipul Rakshit** and Sankar P Sanyal, *Phys. Status Solidi* **B**, 248, Issue-4, 921 (2010).
   Impact factor: 1.489

7. **First-Principles Lattice Dynamical Study of ScAs and ScSb at Zero and High Pressure**
   Bipul Rakshit, Sankar P Sanyal and Massimo Celino, *Solid State. Commun.* **149,** 1326 (2009).
   Impact factor: 1.534

8. **Electronic and elastic properties of alkali-metal sulphides- Li_2S and Na_2S.**
   Premlata Pandit, **Bipul Rakshit** and Sankar P Sanyal, *Indian Journal of Pure and Applied Physics* **47**, 804 (2009).

Impact factor: 0.854

9. **Electronic and Structural Properties of Transition Metal Mono nitrides**
   Poonam Ojha, **Bipul Rakshit** and Sankar P Sanyal, *Indian Journal of Pure and Applied Physics* **46**, 375 (2008).
   Impact factor: 0.854

10. **Lattice Vibrational Properties of Rare-Earth Antimonides: Raman Scattering Measurement and Model Theory**
    Bipul Rakshit, Vipul Srivastava, S P Sanyal, Nita Dilawar, Deepak Varandani and A K Bondyopadhyay, *Journal of Optoelectronic and Advanced Materials* **2 Issue 1**, 37 (2008).
    Impact factor: 0.516

11. **Vibrational Spectroscopy and Phonon Dispersion of GaSb**
    Bipul Rakshit, Vipul Srivastava, S P Sanyal, P K Jha, T R Ravindran and Aklish K Arora, *Indian Journal of Pure and Applied Physics* **46**, 20 (2008).
    Impact factor: 0.854

- **Conference Publications**

1. **A microscopic model for the strain driven direct to indirect bandgap transition in monolayer MoS_2 and ZnO.**
   Ruma Das, **Bipul Rakshit**, Saikat Debnath and Priya Mahadevan, ICONSAT-2014, Punjab, Mohali.

2. **Effects of Vacancies on PtN_2 with Pyrite Structure**
   Bipul Rakshit and Marcos Verissimo-Alves International Conference on the Physics of Semiconductors ICPS 2008 AbstractID: 718-1

3. **Electronic and Elastic Properties of Rock-Salt LaSb from Density Functional Theory**
   Bipul Rakshit and S P Sanyal, DAE SSPS **52** (2007)

4. **Fluorite Structure of Platinum Nitride**
   Bipul Rakshit and S P Sanyal, DAE SSPS **51** (2006) 587

5. **Phonon Dispersion and Vibrational Spectroscopy of GaSb**
   Bipul Rakshit, Vipul Srivastava, S P Sanyal P K Jha, T R Ravindran, and Akhilesh K Arora, DAE SSPS **50** (2005) 629