

**SEMINAR CUM WORKSHOP  
ON FIRST PRINCIPLE  
AND OTHER SIMULATION METHODS  
IN  
CONDENSED MATTER PHYSICS**

**(22-29 March 2010)**

(Organised Under UGC Special Assistance Programme)

Physics Department

Himachal Pradesh University Shimla

**PROGRAMME**

DAY	TIMING	Speakers	Topic
<b>Day 1</b> 22.03.10 (Monday)	<b>Arrival of Participants</b>		
<b>Day 2</b> 23.03.10 (Tuesday)	9.30- 10.30	Registration	
	10.30-11.30 (Inauguration and Key Note Address	Prof. Sunil Gupta , Vice Chancellor, Himachal Pradesh University Prof Sushil Auluck (1) Prof. Emeritus IIT Kanpur	Inaugural address by Hon'ble Vice-Chancellor Keynote address: Computational Material Science
	11.30-12.00		Tea
	12.00-1.30	Prof. GP Das (1) Indian Association for Cultivation of Science Kolkotta	Introductory material on energy bands in solids
	1.30-2.15	Lunch	
	2.15-3.15	Prof. M Harbola (1) IIT Kanpur	Many Electrons Problem: A Precursor
	3.15-3.30	Tea	

DAY	TIMING	Speakers	Topic
	4.00-5.00	Prof. M Harbola (2) IIT Kanpur	Early Attempts to do Many Electron Problem via Density
	5.00-5.15	Tea	
	5.15-630	Prof. PK Ahluwalia (1) HPU Shimla	Preparing for SIESTA
<b>Day 3</b> 24.03.10 (Wednesday)	10.00-11.00	Prof. GP DAS (2) Indian Association for Cultivation of Science Kolkotta	Choice of Basis Sets: Fixed basis vs. Partial Wave methods
	11.00-11.15	Tea	
	11.15-12.15	M Harbola (3) IIT Kanpur	Local Density Approximation and Why It Works
	12.15-01.15	GP DAS (3) Indian Association for Cultivation of Science Kolkotta	Partial Wave Methods
	1.30-2.15	Lunch	
	2.15-3.15	M Harbola (4) IIT Kanpur	Gradient corrections: GEA, GGA and Beyond
	3.15-3.30	Tea	
	3.30-5.00	PK Ahluwalia (2)	SIESTA: An Introduction
	5.00-5.15	Tea	
	5.15-630	PK Ahluwalia (3)	Pre and Post Processing Tools for SIESTA
<b>Day 4</b> 25.03.10 (Thursday)	10.00-11.00	Prof. GP Das (4) Indian Association for Cultivation of Science Kolkotta	Some Applications in Material Science and Nanostructure devices
	11.00-11.15	Tea	
	11.15-12.15	Prof. M Harbola (5) IIT Kanpur	Density functional theory for excited-states

DAY	TIMING	Speakers	Topic
	12.15-01.15	Prof. G.P. Das, Prof. Manoj Harbola, Prof. P.K. Ahluwalia	Question Time
	1.30-2.15	Lunch	
	2.15-3.15	Prof PK Ahluwalia HPU Shimla (4)	Pseudopotential Generation & Testing
	3.15-3.30	Tea	
	3.30-5.00	Dr. Rajiv Kapri (1) IISER Mohalli	Introduction to Monte Carlo Simulations in Classical Statistical Mechanics
	5.00-5.15		
	5.15-6.30	Prof. PK Ahluwalia HPU Shimla (5)	Case studies of Molecules, Metals and Semiconductors Using SIESTA
<b>Day 5</b> 26.03.10 (Friday)	10.00-11.00	Dr. Hitesh Sharma (1) RIEBT Mohalli Panjab Technical University	Functionalized Fullerenes Based Hybrid Nanostructures : An application to Nanotechnology
	11.00-11.15	Tea	
	11.15-12.15	Prof. R Prasad IIT Kanpur (1)	Basics of Classical and Ab-Initio Molecular Dynamics
	12.15-01.15	Dr. Hitesh Sharma RIEBT Mohalli Panjab Technical University	Novel Dilute Magnetic Semiconductors: A Density Functional Study
	1.30-2.15	Lunch	
	2.15-3.15	Dr. Rajiv Kapri (2) IISER Mohalli	Introduction to Monte Carlo Simulations: Two Dimensional Ising Model
	3.15-3.30	Tea	
	3.30-5.00	Dr. Hitesh Sharma RIEBT Mohalli Panjab Technical University	Lab Session SIESTA
5.00-5.15			

DAY	TIMING	Speakers	Topic
	5.15-6.30	Prof. P.K. Ahluwalia (6)	Tutorials LAMMPS
<b>Day 6</b> 27.03.10 (Saturday)	10.00-11.00	Prof. R Prasad (2)	Basics of Classical and Ab-Initio Molecular Dynamics
	11.00-11.15	Tea	
	11.15-12.15	Dr. Hitesh Sharma RIEBT Mohalli Panjab Technical University	Lab Session SIESTA
	12.15-01.15	Dr. Rajiv Kapri (3)	Application of Monte Carlo Simulation: Unzipping of Double Stranded DNA
	1.30-2.15	Lunch	
	2.15-3.15	Prof. P.K. Ahluwalia (7)	Tutorials LAMMPS
	3.15-3.30	Tea	
	3.30-5.00	<b>Visit to Indian Institute of Advanced Study (Rashtrapati Bhavan)</b>	
	5.00-5.15		
	5.15-6.30		
<b>Day 7</b> 28.03.10 (Sunday)	10.00-11.00	Prof. R Prasad (3)	Basics of Classical and Ab-Initio Molecular Dynamics
	11.00-11.15	Tea	
	11.15-12.15	Poster Session/Oral Presentation	Participants Presentation
	12.15-01.15	Panel Discussion: Prof. R Prasad, Prof. Rajiv Kapri, Prof. P.K. Ahluwalia	What Further?
	1.15-2.15	Lunch	
	2.30-3.30	Prof. Chaman Chandan, Dean Of Studies Prof. K.C. Sharma, Prof. Emeritus, HPU	
	Valedictory Function		
3.30 Onwards	High Tea		
<b>Day 8</b> 29.03.10 (Monday)	<b>Departure of Participants</b>		

## **Computational Material Science**

*Prof. Sushil Auluck  
Professor Emeritus  
IIT Kanpur, Kanpur*

### **Abstract**

Computers has seen a tremendous advancement in the past few decades. A history of this advancement will be presented. In particular how this has helped physics will be highlighted. A short discussion of the operating systems will be given. This will be followed by a list of some of the available codes for electronic properties. In the end some results obtained by these codes will be presented.i will inform you about the detailed travel plans later.

## **Basics of Material Simulations**

*Prof. G.P. Das*  
*Indian Association for Cultivation of Science*  
*Jadavpur, Kolkotta*

### **Abstract**

1. **Introductory material on energy bands in solids**  
(Crystal structures, Space groups, k-space, Bloch representation, Energies of electrons in solids, From Bonds to Bands in Solids)
2. **Choice of Basis Sets**  
Fixed basis vs. Partial Wave methods Tight binding theory; Slater-Koster approach Pseudopotential methods
3. **Partial Wave Methods**  
KKR, Muffin-tin orbital (MTO) approach, Linearized Methods : LMTO, LAPW, ASW
4. **Some Applications**
  - (a) Materials Science
  - (b) Nanostructure devices

# Density Functional Theory and Beyond

Prof. MK Harbola  
Physics Department  
IIT Kanpur  
Kanpur

## Abstract

1. **Background:** Many-electron Schrodinger equation; Variational principle; Hartree theory - idea of self-consistency; Hartree-Fock theory, exchange energy; beyond Hartree-Fock, correlation energy (As Hartree and Hartree-Fock theories are discussed, functionals are also discussed)
2. **Early attempts to do many-electron problem in terms of density;** Thomas-Fermi theory and Gradient corrections; Hohenberg-Kohn theorem, Chemical potential; Kohn-Sham formulation; some exact properties of these methods: Janak's theorem, Ionization potential theorem and derivative discontinuity of exchange-correlation potential.
3. **Approximations:** Local density approximation for exchange and correlation - functionals and functional derivatives, understanding why the LDA works; beyond LDA.
4. **Gradient corrections:** GEA functionals; what is physically wrong with the GEA. Going beyond GEA, Generalised gradient approximations (GGA) by Perdew. Becke functional.
5. **Density functional theory for excited-states:** Time-dependent density-functional theory (TDDFT). Time-independent density functional theory: functionals for excited-states.

# **Introduction to Monte Carlo Simulations**

*Dr. Rajiv Kapri  
Physics Department  
Indian Institute of Science Education and Research  
(Camp Office: NITTR, Sector 26, Chandigarh)*

## **Abstract**

In these lectures, we will have an introduction to Monte Carlo simulations in classical statistical mechanics. We will discuss the famous Metropolis and an efficient Wang-Landau algorithm by applying it to the simulation of two-dimensional Ising model. The data analysis methods including standard errors and single and multiple histogram techniques will also be covered. The methods discussed above will be used in the unzipping of a double-stranded DNA by force.

# **Basics of Classical and Ab-Initio Molecular Dynamics**

*Prof. R. Prasad  
Physics Department  
Indian Institute of Technology, Kanpur 208016*

## **Abstract**

During the last few decades molecular dynamics has emerged as a powerful tool to study materials and predict new and exotic materials. In these lectures I shall give an overview of basic foundations of classical as well as ab-initio molecular dynamics with some selected illustrative applications. I shall begin with the classical molecular dynamics which uses Newton's equations of motion to obtain atomic trajectories. For illustration I shall use a system of interacting particles interacting with the Lennard-Jones potential. I shall show how one can obtain quantities such as diffusion coefficient and phonon densities of states by analyzing the time-dependence of root-mean square displacement and velocity-auto correlation function. I shall then move to the discussion of ab-initio molecular dynamics using the Born-Oppenheimer approximation. The advantage of ab-initio MD over classical MD is that it does not use any empirical potential or any adhoc parameter. The forces between the atoms are obtained using the Density Functional Theory. The basic equations of Car-Parrinello molecular dynamics will be derived. The ideas of simulated annealing and steepest descent will be discussed. I shall briefly discuss how it can be implemented using the plane-wave expansion method. Then I shall show how the Car-Parrinello molecular dynamics can be used to predict cluster geometries by giving some examples. Finally, the application of this method to generate amorphous structure and to study hydrogenated amorphous silicon will be discussed.

# **Functionalized Fullerenes Based Hybrid Nanostructures**

## **An application to Nanotechnology**

Dr. Hitesh Sharma  
Department of Applied Sciences  
RBIEBT, Sahauran, Mohali (Punjab Technical University, Jalandhar)

### **Abstract**

The functionalized carbon nanostructures have shown many tailorable novel properties which can be exploited for possible application in future nanotechnologies. In this presentation, role of selective doping by N and B in fullerenes to tune its electronic properties will be discussed along with its application to make molecular devices. The extra stability of  $C_{60}$  can be used for encapsulation of many elements which may lead to possible energetic materials. The role of transition elements in introducing magnetism in fullerene endohedral complexes will be discussed. The catalytic properties of the fullerenes, which varies as function of curvature will also be discussed for improving kinetics of the metal hydride complexes important for realization of the solid state hydrogen storage.

# **Novel Dilute Magnetic Semiconductors: A Density Functional Study**

Dr. Hitesh Sharma  
Department of Applied Sciences  
RBIET, Sahauran, Mohali (Punjab Technical University, Jalandhar)

## **Abstract**

Magnetic semiconductors are recently considered as one of the main building blocks for future replacement of conventional electronics by spintronics. Presently, there have been lot of efforts to produce dilute magnetic semiconductors (DMSs) with Curie temperature above room temperature. DMS is usually produced by doping semiconductors by transition metals (TMs). The room temperature has been reported in semiconductors from group-IV and II-VI. In the present talk the implication of Cr doped Germanium clusters exhibiting high spin state, can be studied for future spintronics applications. The role of the co-doping will also be discussed for improving stability and magnetic properties. Secondly, the role of the C doped ZnO system as potential dilute magnetic semiconductor will be discussed. Till recently, the TM doped ZnO systems were considered as a strong material for spintronics but is poorly understood. The origin of the observed FM continues to be strongly debated. The presence of intrinsic defects such as Zn vacancy or O vacancy has also been attributed to largely unexplained source of magnetic properties. It will be interesting to include the role of C distribution and point defects in carbon doped ZnO (ZnO:C) systems.

# **Siesta Applications-I: Structural, vibrational and electronic properties of nanoclusters**

**Case study:  $Al_n$  and  $Al_nN$  clusters**

*Dr. Hitesh Sharma*

*Department of Applied Sciences*

*RBIEBT, Sahauran, Mohali (Punjab Technical University, Jalandhar)*

## **Abstract**

In this Session, application of siesta to determine the structural, vibrational and electronic properties of pure and binary nanoclusters shall be discussed. The issues to be addressed are as follows:

1. To understand and define problem using siesta.
2. To decide on the choice of simulation parameters for a particular problem.
3. To set the test calculations and exchange correlation functions.
4. Search for the global minimum structures.
5. Calculate structural, electronic and vibrational properties.

## **Siesta Applications-II: Structural and Electronic Properties of Carbon Nanostructures**

**Case study: Fullerenes, Azafullerenes and Carbon Nanotubes**

*Dr. Hitesh Sharma and Isha Garg*

*Department of Applied Sciences*

*RBIEBT, Sahauran, Mohali (Punjab Technical University, Jalandhar)*

### **Abstract**

In this Session, application of siesta to determine the structural and electronic properties of carbon nanostructures such as fullerenes, azafullerenes and carbon nanotubes shall be discussed. The issues to be addressed are as follows:

1. To understand and define problem using siesta.
2. To decide on the choice of simulation parameters for a carbon nanostructures.
3. To set the test calculations and exchange correlation functions.
4. Search for the global minimum structures.
5. Calculate structural and electronic properties.

# Simulations of Large Scale Simulations Using Open Source Codes: SIESTA and LAMMPS

*Prof. P.K. Ahluwalia  
Solid State Theory Group  
Physics Department  
Himachal Pradesh University  
Shimla*

## **Abstract**

A world wide impetus to the study of classical and quantum materials has resulted with the availability of open source codes which can be run on serial and parallel machines. Two such codes namely SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) and LAMMPS (Large Scale Atomic/Molecular Massively Parallel Simulator) are the biggest open source efforts which have facilitated the study of quantum and classical materials in a big way.

Following five tutorials to run first principle calculations using SIESTA Code will be presented in LINUX environment through an exploratory approach to have a peep into the intricacies of the code to study a variety of physical systems such as molecules, bulk, surfaces and wires using localized atomic orbitals in contrast to computationally costly plane wave methods:

- Preparing for SIESTA
- SIESTA: An Introduction
- Pre & Post Processing Tools for SIESTA
- Abinitio Pseudopotential Generation and Testing
- Case Studies of Molecules, Bulk Systems (Metals, Semiconductors and Complex structures) Using SIESTA

Following two Tutorials will be conducted to have an understanding of Classical Molecular Dynamics through LAMMPS an open source code.

- LAMMPS: An Introduction
- LAMMPS: Case Study for Mono and Binary Liquids

These tutorials have been built to supplement the basics of First Principle and Molecular Dynamics calculations being covered in the present Seminar cum Workshop.

**LIST OF PARTICIPANTS WITH POSTAL AND E-MAIL ADDRESSES**

S. No.	Name		Institution/ Permanent Address	e-mail
1.	Dr Anil Thakur	HPU	Physics Deptt HPU Shimla/ Anil Bhawan, Hospital Approach Road Solan	<a href="mailto:Anil_t2001@yahoo.com">Anil_t2001@yahoo.com</a>
2.	Brij Mohan	HPU	Physics, Deptt. HPU SHIMLA/ Ph. D.Scholar, Physics Department, HPU Shimla.	<a href="mailto:brijmohanhpu@yahoo.com">brijmohanhpu@yahoo.com</a>
3.	Arun Kumar	HPU	Physics, Deptt.HPU SHIMLA/ Ph. D.Scholar, Physics Department, HPU Shimla	<a href="mailto:arun242493@yahoo.com">arun242493@yahoo.com</a>
4.	Renu Kumari	HPU	Physics, Deptt. HPU SHIMLA/ Ph. D.Scholar, Physics Department, HPU Shimla.	<a href="mailto:renu279048@yahoo.com">renu279048@yahoo.com</a>
5.	Ranjan Kumar	PU	Deptt. Of Physics Lecturer, Deptt. Of Physics, Panjab University, Chandigarh- 160014.	<a href="mailto:ranjan@pu.ac.in">ranjan@pu.ac.in</a>
6.	Rahul Tripathi	NPL	St. Johns College, Agra/ SRSA-26, Ind Floor, NPL Colony, New Rajendra Nagar, New Delhi.	<a href="mailto:tripathir@mail.nplindia.org">tripathir@mail.nplindia.org</a>
7.	Devina Sharma	NPL	Panjab University/ Room No.109, Main Building, National Physical, Lab CNPL Pusa Campus, New Delhi-110012	<a href="mailto:Sharmadevina@yahoo.com">Sharmadevina@yahoo.com</a>
8.	Jagdish Kumar	NPL	HPU Shimla 3/2 JRF Hostel, NPL Colony, New Rajinder Nagar, New Delhi- 110060.	<a href="mailto:jagdishphysicist@gmail.com">jagdishphysicist@gmail.com</a>
9.	M.Hemandhan	IITK	Department of Physics, IIT Kanpur, Kanpur U.P-208016	<a href="mailto:hemanadh@iitk.ac.in">hemanadh@iitk.ac.in</a>
10.	Sheetal Sharma	PU	Roll no-51,Room no.70, Girls Hostel no-2 P.U Chandigarh.	<a href="mailto:Shetal4984@gmail.com">Shetal4984@gmail.com</a>
11.	Pooja Rani	PU	Deptt of Physics, P.U. Chandigarh.	<a href="mailto:poojagoyal0510@yahoo.com">poojagoyal0510@yahoo.com</a>
12.	Ashutosh Sharma	IIT	A-108 Hall-7 IIT Kanpur, Kanpur 208016	<a href="mailto:Atsharma@iitk.ac.in">Atsharma@iitk.ac.in</a>
13.	Renu Thakur	HPU	Deptt. Of Physics H.P.U Shimla – 171005.	<a href="mailto:renuthakur81@gmail.com">renuthakur81@gmail.com</a>
14.	Shanta	HPU	Deptt of physics H.P.U Shimla.	<a href="mailto:shantakapoor@gmail.com">shantakapoor@gmail.com</a>
15.	Ashok Kumar	HPU	Deptt. Of physics, H.P.U. Shimla 171005	<a href="mailto:ashok1777@yahoo.com">ashok1777@yahoo.com</a>
16.	Babita Rani	PBIU	Lecturer, Physics, Deptt. Punjabi University, Patiala-147002	<a href="mailto:babitabaghla15@gmail.com">babitabaghla15@gmail.com</a>
17.	MD. Shamim	IITK	Deptt. of Physics IITkanpur, Kanpur. U.P. PIN- 208016	<a href="mailto:sami@ii+kac.in">sami@ii+kac.in</a>
18.	Sonu Kumar	IIT	Jwalamukhi Hostal, D-23, Hauz- khas, New Delhi, Pin-110016.	<a href="mailto:1009ukumar@gmail.com">1009ukumar@gmail.com</a>
19.	Rinki Dhingra	IIT	Deptt. Of Physics/Cabin No. 15 Research Scholar's Room-I IIT	<a href="mailto:rinky.phy@gmail.com">rinky.phy@gmail.com</a>

S. No.	Name		Institution/ Permanent Address	e-mail
			Roorkee/PIN-247667.	
20.	Sanjeet Kumar	NPU	N.P. University/Qtr. No. RKI-326, Roarahbandh, P.O. Sindri, Distt. Dhanbad Jharkhand-828122	<a href="mailto:san.phy18@gmail.com">san.phy18@gmail.com</a>
21.	Vibhav Pandey	NPL	National Physical Laboratory, Room No. 120, Magnetic standards main building, K.S. Krishnan Marg New Delhi-1100.	<a href="mailto:vibhavpandey18@gmail.com">vibhavpandey18@gmail.com</a>
22.	Karandeep	IITN	IIT Delhi, Shivalik Hostal, SA-20 Hauz-Khas, New-Delhi-110016	karandeepster@gmail.com
23.	Anup Kumar	GCHPU	Govt.Degree.College. Kullu.	kumar.anup.sml@gmail.com
24.	Amritendu Roy	IITK	Department of Material and Metallurgical, Engineering Indian Institute of Technology, Kanpur-208016 Uttar Pradesh; India	tendu@iitk.ac.in
25.	Sanjeev Kumar	PCHPU	Physics Deptt. , St. Bede's College, Shimla 171002 H.P.	sk_06 indiatimes.com
26.	Rohan Samkaria	NIT	Deptt. of Physics, NIT-Hamirpur (H.P.) Pin.-177005.	rohan_samkaria@rediffmail.com
27.	Dr. Kuldeep Kumar Sharma	NIT	Asstt. Prof., Department of Physics, NIT Hamirpur (H.P.) Pin.-17700.	kks@nitham.ac.in & kknitham@gmail.com
28.	Dr. Vimal Sharma	NIT	Deptt. Of Physics NIT Hamirpur Pin.-177005.	vimal k sharma@yahoo.co.in
29.	A.H.M Abdul Wasey	IACS	Deptt. Of Materials Science, Indian Association for the Cultivation of Science, Kolkata-700032.	msaaw@iacs.res.in
30.	Amrita Bhattacharya	IACS	Deptt. of Material Science, IndianAsociation for the Cultivation of Science, KolkataPin.-70032.	msab2@iacs.res.in
31.	Ramandeep	IITR	F-48 Kasturba Bhawan IIT roorkee.	<a href="mailto:Rmn_bhlr@yahoo.com">Rmn_bhlr@yahoo.com</a>
32.	Mrs. Shobhna Dhiman	PEC	Sr. Lecturer, PEC University of Technology, Chandigarh-160012.	<a href="mailto:s-dhiman@hotmail.com">s-dhiman@hotmail.com</a>
33.	Saswata Bhattacharya	IACS	Deptt. of Material Science, Indian Association for the Cultivation of Science Kolkataa-700032.	<a href="mailto:mssb3@iacs.res.in">mssb3@iacs.res.in</a>
34.	Nalini Sharma	HPU	Nalimi Sharma Department Of Physics H.P. University Shimla-5.	<a href="mailto:nalini_2808@yahoo.co.in">nalini_2808@yahoo.co.in</a>
35.	Sanvane Yogesh Kumar	SGU	Deptt. of Physics Veer Narmad South Gujarat University, Udhina-Magdalla road Surat-395007.	<a href="mailto:yogesh126@gmail.com">yogesh126@gmail.com</a>
36.	Surjeet Kumar Chandel	GCHPU	Govt. P.G. Collage Bilaspur(H.P.)	<a href="mailto:skchandel2@yahoo.co.in">skchandel2@yahoo.co.in</a>
37.	Satish Kumar Chandel	HPU	H.No. E-2, Collage Colony Bilaspur, (H.P.)-174001.	<a href="mailto:satish Chandel@gmail.com">satish Chandel@gmail.com</a>
38.	Avneesh Kumar	^HPU	VPO: Takrera, Distt. Bilaspur, H.P. 174021.	<a href="mailto:avneesh76@yahoo.co.in">avneesh76@yahoo.co.in</a>
39.	Ishu Goyal	PU	Deptt. of Physics, Punjab University, Chandigarh-160014.	igoyal 1986 @ gmail.com
40.	Ganan Preet	PU	Deptt. Of Physics, Punjab University, Chandigarh, Pin Code-160014, India.	gaganprt93@gmail.com
41.	Renu Bala	PU	H. No. 538-A New Police Colony Sector-26 Chandigarh-160019	renu28feb@gmail.com

S. No.	Name		Institution/ Permanent Address	e-mail
42	Shyam Kumar G. Khambholja	SPUG	Magadev vali Gali, NR vaniya devi, Dakaor 388225 District Kheda Gujrat	physik.shyam@gmail.com
43	Dr. JD Sharma	SUHPU	Physics Department, Shlooni University, Solan	sharmajyotid@gmail.com
44	Dr. R. K. Modgil	KUK	Physics Department Kurukshetra University, Kurukshetra	rkmoudgil13@gmail.com
45	Monika Dhaliwal	GJUST	Physics Department G. J. U. S. &T Hissar	<a href="mailto:Monikadhariwal9@gmail.com">Monikadhariwal9@gmail.com</a>
46	Leena	PUP	Physics Department Panjabi University Patiala, PB	<a href="mailto:leena-physics@yahoo.com">leena-physics@yahoo.com</a>
47	Shivali Sharma	PUP	Physics Department Panjabi University Patiala, PB	<a href="mailto:sharma_shivali05@yahoo.com">sharma_shivali05@yahoo.com</a>
48	Isha Garg	PUC	Deptt. Of Physics, Punjab University, Chandigarh, Pin Code-160014, India.	ishagarg.pu@gmail.com