Name	Dr. Anjali Kshirsagar
Qualification	M.Sc. Ph.D. (Physics)
Designation	Reader
Specialization	Computational Condensed Matter Physics
Email	anjali@physics.unipune.ernet.in
Phone	020 25699072 extn 317

1 Education

	Course	Institution	Year
1	B.Sc.	Holkar Science College, Devi Ahilya VishwaVidyalay, Indore	1976
2	M.Sc. (Physics)	Department of Physics, University of Pune, Pune	1978
3	Ph.D. (Physics)	Department of Physics, University of Pune, Pune	1985

2 Career Profile

	Organisation / Institution	Designation	Duration
1	Department of Physics, Univer	Joined as a Lecture	since 1986
2			
3			

3 Teaching Experience (Subjects/Courses Taught) 22 yrs

Methods of Mathematical Physics, Quantum Mechanics, Numer

4 Research Interests / Specialization

Electronic Structure of Bulk and Nanostructures, Materials Mode

5 Honors & Awards

Senior Group Associate of Abdus Salam International Centre fo

6 Publication - Books, Journals, Articles

	Year of Publication	Title	Co-Author

1	2008	ECR plasma assisted deposition of zinc nanowires	V.S. Purohit, S. Dey, Somesh Kr. Bhattacharya,C.V. Dharmadhikari and S.V. Bhoraskar
2	2008	Electronic structure of GaN codoped with Mn and Cr	Nandan Tandon, G.P. Das
3	2008	Passivation of CdTe clusters : A first principle study	Somesh K. Bhattacharya
	2008	Empirical pseudo-potential studies on electronic structure of semiconducting quantum dots	Neelesh Kumbhojkar
	2007	How cationic gold clusters respond to a single sulfur atom	Hagos W.Ghebriel
	2007	Adsoption of molecular hydrogen and hydrogen sulphied on Au cluster	Hagos W.Ghebriel
	2007	Ab initio calculations of the structural and electronic properties of CdTe clusters	Somesh K. Bhattacharya
	2006	Electronic structure of diluted magnetic semiconductor $Ga_{1-x}Mn_xN$ and $Ga_{1-x}Cr_xN$	Nandan Tandon, G.P. Das

	2005	Momentum-space properties from coordinate-space electron density	Manoj K. Harbola, Rajendra R. Zope, Rajeev K. Pathak
	2001	Optical properties of II-VI semiconducting quantum dots	Neelesh Kumbhojkar
	2000	Photophysical properties of ZnS nanocrysta	Neelesh Kumbhojkar , V.V. Nikesh, Shailaja Mahamuni
	2000	Full-potential LAPW calculation of electron momentum distribution of ferromagnetic Ni	Tunna Baruah, Rajendra R. Zope
	1999	Full-potential LAPW calculations of electron momentum density and related properties of Li	Tunna Baruah, Rajendra R. Zope
	1997	Density functional approach to one positron and neutral atom bound state	Tunna Baruah, Rajeev K. Pathak
	1995	Leading corrections to the Compton profiles beyond the impulse approximation : second-order correction	Rajendra R. Zope, Rajeev K. Pathak,

	1996	Evidence of size independent electronic structure : BaO particles in nanosize regime	Shailaja Mahamuni, B.S. Bendre, Tunna Baruah, S.S. Joshi, A.G. Bedekar, S.F. Patil, P. Singh, K. Maiti, D.D. Sarma
	1994	Positron binding : A positron density viewpoint	Tunna Baruah, Rajendra R. Zope, Rajeev K. Pathak
	1993	Leading corrections to atomic impulse-approximation Compton profiles : A density functional approach	Rajeev K. Pathak, Ruth Ho meyer, Ajit J. Thakkar
	1993	Thiophenol-capped ZnS quantum dots	Shailaja Mahamuni, Ali Azam Khosravi, Manisha Kundu, Anjali Bedekar, D.B. Avasare, Prabhat Singh and S.K. Kulkarni
	1990	Present status of the Compton profile calculation in transition metals	V. Sundararaja n, D.G. Kanhere,
	1989	Two-component density functional theory of positron binding to negative ions	D.G. Kanhere, Vasudha Bhamre,

	1989	Fourier transform of momentum density in Pd and PdH	D.G. Kanhere, R.M. Singru,
	1988	Compton profile of Palladium	B.K. Sharma, Anil Gupta, Hanuman Singh, S. Perkki¨o, D.G. Kanhere,
	1986	Two photon momentum density and angular correlation of positron annihilation radiation in Pd and PdH	D.G. Kanhere, R.M. Singru
	1985	Calculation of 1D- and 2D-angular correlation curves in Pd and PdH	D.G. Kanhere, R.M. Singru
	1985	Electron momentum distribution in Pd and PdH	D.G. Kanhere, R.M. Singru
	1983	Momentum space properties of atoms	Alfredo M. Simas, Vedene H. Smith, Jr., William M. Westgate
	1982	Compton profiles for neon and argon from X♋ wavefunctions	P.V. Panat, D.G. Kanhere
	2006	Book for Science for Class IX of Secondary Board of Maharashtra	Sushama Joag, Ramesh Patil, Badrinaraya n Kabra
	2007	Book for Science for Class X of Secondary Board of Maharashtra	Sushama Joag, Manisha Kulkarni,Sak haram Aghav

	2007	Physics Book for Class XII of Central Board	

7 Publication - Conference Presentations

1. Theme Meeting on Materials Modeling @ Different Length Scales (MMM-2006) held
2. Round Table Meeting on the Science of Processing Plasmas held at Bhabha Atomic
3. Meeting on Condensed Matter Physics held at S. N. Bose National Centre for Basic
4. First Conference of Asian Consortium for Computational Materials Science held at B
5. National Conference on Science & technology of Nanomaterials & Clusters held at B
6. SERC school on Electronic Structure Calculations held at SNBNCBS, Kolkata, India
7. Conference on Electronic Structure and Physics of Materials held at SNBNCBS, Koll
8. Workshop on Novel Directions in Quantum Mechanics and Materials Science held a
9. Workshop on The Physics of the Electronic Behavior in Core Region : all-electron LA
10. Fourth International Conference on Nanostructured Materials (NANO 98) held at St
11. APW calculation of positron angular correlation in Pd and PdH, Paper presented at
12. Discussion Workshop on Electronic Structure and Phase Stability of Alloys held at
13. Sixth International Conference on Positron Annihilation held at Fort Worth, Texas, U

8 Professional Societies Memberships

*** Member and Chartered Physicist, Institute of Physics (UK)**
*** Life member of Indian Physics Association**
*** Life member of Indian Association of Physics Teachers**
*** Life member of Marathi Vidyan Parishad, a body with about 1000 life members, v**
*** Member of the Third World Organization for Women Scientists.**

9 Public Service / University Service / Consulting Activity

10 Projects (Major Grants / Collaborations)

1. Coordinated Research Project on Spintronics funded by Board of Research in
2. Tight Binding Molecular Dynamics Simulations for Semiconductor Nanocrystal
3. Feasibility study of tailoring of Diluted Magnetic Semiconductor (DMS) materia
4. Electronic Structure of Doped Semiconductor Nanoclusters funded by Univer
5. Feasibility Study of Nanoaluminium in HTPB and DOA Matrix funded by Arman
6. Electronic Structure of Diluted Magnetic Semiconductor $Cd_{1-x}Mn_xTe$ funded by
7. Highly Accurate Studies of Electron momentum distributions in simple metals
8. Electron Momentum Distributions in Transition Metals and Their Compounds ,
9. Electronic structure of 2-D array of GaAs nanocrystals , funded by Board of Re
10. Size dependence of the electronic structure of II VI semiconductor quantum d
11. Car-Parrinello method of molecular dynamics with augmented plane wave bas
12. Some investigations on atoms, molecules and solids in position and momentu

11 Other Details

(a) Research Supervised
Ph. D.s awarded :

1. “LAPW studies of Electron Momentum Distributions and Related Properties in Solic
2. “Studies on Atomic Systems in Coordinate and Momentum Spaces within Density F
3. “Studies of Size Dependence of the Electronic Structure of Semi-conducting Quantu
4. “Synthesis and Characterization of Zinc Oxide Quantum Dots” , Bhausaheb Bendre,

5. “Density Functional Study of Electronic and Structural Properties of Different Gold Cluster complexes”, Hagos W. Ghebriel, from Ethiopia, degree awarded in October, 2008.

M.Phil.s awarded :

1. “Positron Binding with Atoms and Ions”, Tunna Baruah, degree awarded in March,
2. “Electronic Structure Studies of very small Clusters of ZnS”, Sanjay Shete, degree av
3. “Electronic Structure and Geometries of Small Mn_x and Mn_x Clusters”, Meena Vidhale, degree awarded in December, 2007

Ph. D.s ongoing

1. “Studies of Electronic structure and Magnetism in Transition Metal Doped GaN and
2. “Density Functional and Tight Binding Simulation Studies of II-VI Semiconductor Clu
3. “Realistic Tight Binding and First Principles Calculations for CdS Clusters” : Prajakta
4. “Molecular Dynamics of Nanoclustures” : Dattatraya Lalsare
5. “Electronic Structure and Optical Properties of Semiconductor Nanocrystals” : Heyd

Research Interests / Specialization

I have expertise in computational condensed matter physics with focus on electronic s

A brief description of some of the work follows : (a) Plane Wave Psuedopotential met

We have studied the smallest cage-like structure of Cd9S9 doped with varying numbe

We have investigated small neutral and cationic gold clusters to understand their frag

(b) Tight Binding Theory for Semiconductor nanostructures : Tight Binding (TB) progra

(c) Diluted Magnetic Semiconductors : Diluted magnetic semiconductors (DMS) are ex

Co-doping ofMn and Cr, which incorporates the salient features typical of both transit

(d) Electron Momentum Distributions and Compton Scattering Studies Interest in Com

Extension

I have been actively working for popularization of science especially physics and comp

I write scientific articles at popular level in newspapers in regional languages, write sc

Details
Gold Medalist, Third in the Order of Merit in the University

ical Analysis, Statistical Mechanics,Solid State Physics

eling

r Theoretical Physics, Trieste, Italy

Book/Journal/Article

Nucl. Inst. Methods in Phys. Res. B 266, p. 4980

Phys. Rev. B 77, p. 205206

Eur. Phys. J. D 48, p. 355

Bull. Mater. Sc. 31, p. 297 Special issue on Nanoscience and Nanotechnology

J. Chem. Phys. 127, p. 224708

J. Chem. Phys. 126, p. 244705

Phys. Rev. B 75, p. 035402

J. Phys. : Condens. Matter 18, p. 9245

J. Chem. Phys. 122, p. 204110

In a book Science and Technology of Nanostructured Materials, edited by B.K. Rao, S.M. Bose, M.P. Das ar

J. Appl. Phys. 88, p. 6260

Phys. Rev. B 62, p. 16435

Phys. Rev. B 60, p. 10770

Phys. Rev. A 55, p. 1518

Chem. Phys. Lett. 242, p. 555

NanoStructured Materials 7, p. 557

Phys. Rev. A 50, p. 2192

Phys. Rev. A 48, p. 2946

J. Appl. Phys. 73, p. 5237

in Positron Annihilation and Compton Scattering edited by B.K. Sharma, P.C. Jain and R.M. Singru, Publishe

Chem. Phys. Lett. 160, p. 526

in Positron Annihilation edited by L. Dorikens-Vanpraet, M. Dorikens and D. Segers and published by World

Phys. Rev. B 37,p. 6821

Phys. Rev. B 34, p. 853

in Positron Annihilation edited by P.C. Jain, R.M. Singru and K.P. Gopinathan, Published by World Scientific

Phys. Rev. B 31, p. 6415

Int. J. Quantum Chem. vol. XXIII,p. 811

J. Phys. B 13, p. 3075

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at Bhabha Atomic Research Centre (BARC), Mumbai during October 12-14, 2006.
: Research Centre (BARC), Mumbai during July 6-7, 2006
Science (SNBNCBS), Kolkata, India during March 10-11, 2006.
Bangalore, India during November 29 - December 1, 2001
Bhopal, India during November 23-25, 2000.
during November 15-19, 1999.
kata, India during November 21-22, 1999.
t Department of Physics, University of Pune, India during December 7-17, 1998.
LPW Electronic Structure Calculations held at AS ICTP, Trieste, Italy during June 22 - July 4, 1998.
tockholm, Sweden during June 14-19, 1998.
the Sixth International Conference on Positron Annihilation held at Fortworth, Texas, USA in April, 1982.
SNBNCBS, Calcutta, India during April 23-26, 1996
JSA during April 3-7, 1982.

Working for Science in State language.

Nuclear Sciences, Government of India. This is a unique project funded by BRNS and involves 10 pe
ls funded by Department of Science & Technology, Government of India, Duration : June, 2005 to Ju
ls with Tc around room temperature funded by ISRO-UoP Space Technology Cell, University of Pune
sity of Pune. Duration : June 2006 to June 2008.
nent Research Board, DRDO, Government of India. Duration : November, 2004 to March, 2006.
Board of Research in Nuclear Sciences, Government of India under the BARC-PU MoU, August, 200
and their compounds , funded by University Grants Commission, Government of India under the Re-
funded by University Grants Commission, Government of India. Duration : April, 1999 to December, 2
search in Nuclear Sciences, Government of India. Duration : June, 1995 to June, 1998.
ots : experiment and theory , funded by Department of Science & Technology, Government of India. D
sis set , funded by Department of Science & Technology, Government of India. Duration : October, 19
um spaces using reduced, first order atomic and molecular density matrices , funded by University G

ds” , Tunna Baruah, degree awarded in February, 2000.
Functional based Theories” , Rajendra Zope, degree awarded in March, 1999. (coguide)
um Dots” , Neelesh Kumbhojkar, degree awarded in April, 2002.
, degree awarded in October, 2003. (co-guide)

1995
warded in November, 1998

CdTe” : Nandan Tandon
sters” : Somesh Bhattacharya
Deodhar

der Ali Shafiei Gol

structure methods based on density functional theory to study condensed matter. The work carried out till

hod for clusters : Currently we have been performing density functional based calculation using ab initio ps

r of Mn atoms. The smallest stable stoichiometric cage-like structure Cd9S9 of CdnSn is found to have enou

mentation path ways and adsorption. Minimum energy structures of neutral and cationic Au(0/+) n (n = 1 -

m package is currently being developed. Computationally, it lies between the first principles methods and

pected to play an important role in spintronics , an upcoming field which exploits both the spin and the ch

ion metal atoms has been tried to tailor a suitable system for DMS applications. This is the first such study

npton scattering research has been revived in last 6-8 years due to availability of better experimental resol

puter science amongst school and college students since 1979. I have worked as an Executive Committee m

ripts for science programmes at All India Radio and deliver lectures on topics of current interest in physics

ıd S.N. Sahu, Published by Nova Publishers

ed by Omega Scientific Pub.

Scientific Co., p. 236.

Co., p. 294.

rsons from 6 different institutes in the country. The aim is to make substantial contribution in the f
ne, 2008.
. Duration : August, 2007 to August, 2008.

3 to August, 2008.
search Award scheme. Duration : March, 2002 to March, 2005.
2001.

Duration : April, 1994 to December, 1997.
93 to June, 1996.
rants Commission, Government of India. Duration : March, 1992 to March, 1995.

l now is based on state-of-the-art first-principles methods to study real-space and momentum space pro

seudopotentials (PAW / USPP) to simulate the lowest energy structures of II-VI semiconductor clusters a

ugh space to dope atoms endohedrally. Single Mn doped cage is formed with a magnetic moment of 5 n

- 8) are found to be two-dimensional. The lowest energy structures of neutral gold clusters are planner a

empirical methods but is preferred for accuracy as it takes into account explicitly the quantum mechani

ıarge degrees of freedom of an electron. However, the current devices based on DMS are functional onl

in GaN and it proposes a better possible spintronics material with known band gap and Tc. The study ca

utions for measuring the electron momentum distributions and increased computational power in recer

ıember in various capacities for the Indian Physics Association since 1979. We also coordinate various ac

in English or regional languages for students and teachers in schools and colleges.

ield of spintronics from India both in Basic understanding of the materials involved and in device a

›perties for atoms and solids. Many of the necessary program packages for the work have been develop

ınd noble metal clusters. These materials display unusual structural and electronic properties for lower c

ıuB but bi-doped endohedral cage is unstable. We substitutionally doped the cage with n Mn atoms wit

after H2 or H2S adsorption but the cationic gold clusters transform into three-dimensional structures at

cal electronic interaction of the system. TB approach is suitable for handling large systems compared to

y at low temperatures as a consequence of their low Curie temperatures (Tc). The key for achieving prac

n provide impetus for experiments to make tailor-made materials for device applications.

nt years. We have employed Full potential LAPW method to calculate the Compton profiles (CP) and pos

ctivities for physics teachers outside our Department to promote physics teaching. The activities of the A

applications.

ed in my research group.

dimensions. In II-VI semiconductor clusters surface reconstruction, formation of cleavage planes and dop

h n = 1-9. Mn substituting S is found to be a less favorable geometry than Cd substitution. On the other h

n = 7 and at n = 3 for cationic clusters of gold with sulfur. The adsorbed molecules get adjusted such tha

methods based on plane wave basis. For nano clusters, which lack periodicity of the lattice, a real space

ctical applications of such devices is to synthesize high-Tc ferromagnetic DMS and consequently to unde

itron angular correlation curves in Li, Fe, Ag etc. Our results agree with the available experimental result

Association's Pune Chapter gained momentum during my tenure as a Secretary and the association is no

ɔing of transition metal impurity atoms are other interesting properties. The HOMOLUMO gap for these

hand, substitutional doping is energetically favored than endohedral doping for n = 1. The magnetic mor

t their centers of mass lie on the plane of the gold cluster. Hydrogen sulphide adsorbed clusters with od

electronic structure calculation is recommended. More realistic sp3d5 basis with nearest and next near

rstand the origin of the ferromagnetism in DMS. First principles electronic structure calculations are wa

ts after applying the Lam-Platzman correction. Inclusion of GGA is found to have significant e ect on the

w recognized and appreciated even outside the physics community. I was instrumental in installing vari

clusters can be tuned by changing the shape, size and by doping impurities. These also constitute impor

ment of the cage is 5n μB up to n = 7. For larger values of n, the magnetic interactions decrease the tota

d number of gold atoms are more stable than the neighboring even n clusters. Such studies are importa

'est interactions included is employed to study medium sized clusters of II-VI semiconductors.

rranted to make definitive statements re warranted to make definitive statements

spin momentum density in Ni, magnetic Compton profiles are compared with experiments. Recently, Cc

ous awards for under-graduate, post-graduate and research students and college teachers through the A

tant materials from device application point of view viz. LEDs, sensors etc. Analysis of the structural pro

l magnetic moment of the cluster. Doping with other transition metal atoms also depicts similar results.

nt since nano gold wires are used in connections for nano devices and gold clusters are also known to be

ompton scattering experiments have been carried out at low-temperatures and with low incident energi

Association.

perties is important to understand the evolution of the geometric structure. The initial geometries of nc

e good catalysts in certain reactions. Density of states and charge density analyses together help to qual

es for Li. We have calculated temperature-dependent CP. A comparison with experiments brings out the

ɔnstoichiometric clusters were considered as fragments of the bulk with Td symmetry. It was observed t

itatively understand electron transport in clusters, this is useful in single electron devices and in sys

e importance of such studies. We have extended the state-of-the-art band structure code to calculate th

hat up

ıe CP and the code is bei