Final Project Report of UGC Major Research Project for the Period

29th October, 2014 to 05-04-2021

"Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory"

No. F. 42-861/2013 (SR)

Dated: **29th October 2014**

submitted to

UNIVERSITY GRANTS COMMISION
BAHDURSHAH ZAFAR MARG
NEW DELHI – 110022

By

Dr. Minal H. Patel(Principal Investigator)
Dr. J.K. Baria(C0 – Investigator)
Associate Professor in Physics,
Department of physics
V.P. & R.P.T.P. Science College,
Vallabh Vidyanagar – 388120
GUJARAT

VRSC/2021-22/52

From: Dr. M. H. Patel,
Associate Professor in Physics,
V. P. & R. P. T. P. Science College,
Vidyanagar - 388 120
Email: mhp67@rediffmail.com
5th May, 2021

To,
The Secretary,
University Grants Commission,
BAHADUR SHAH ZAFAR MARG
NEW DELHI - 110 002

Sub: UGC Major Research Project No. **F. 42-861/2013 (SR)** dated **29th October 2014** Final Project Completion report ...

Dear Sir,

I have received the UGC Major Research Project No. **F. 42-861/2013 (SR)** dated **29th October 2014** entitled: **"Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory".** This project has been successfully completed and all completion documents have been submitted to UGC New Delhi.

I am submitting the detail of the research activity including publication, participation in seminar and conferences as well as the utilization of grant under various heads such as books & journals, Equipment, contingency travel and field work.

I therefore request you to acknowledge the receipt of the letter and settled the account to close the project. **I also request you to issue me the project completion certificate earliest.**

With thank and regards.

Sincerely Yours,

Dr. Minal H. Patel
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar - 388 120

Dr. J.K. Baria
(Co-Investigator)
Associate Professor in Physics,
V P & R P T P Science college,
Vallabh Vidyanagar - 388 120

Enclosed:
1. UGC Major Research Project Completion Certificate (PCR).
2. Uploading project detail on our college website Certificate.
3. All annexure's (Annexure III to Annexure XII) including Evaluation report.
4. Reprint of all research papers and conferences attended.
5. Soft copy of final report in CD.
6. RTGS/NEFT acknowledgement slip of Unspent amount Rs. 2,50,112/- deposited to UGC Account.

Project Completion Report (PCR)

Certified that the Major Research Project entitled: **"Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory"**, No. **F. 42-861/2013 (SR)** dated **29th October 2014** awarded to **Dr. Minal H. Patel(PI)** and **Dr. J.K. Baria(CI)** of this college, in the subject of **Physics** has been successfully completed and all completion documents have been submitted to UGC New Delhi.

Dr. Bhavesh Patel
Signature of the Principal
With seal of the college

PRINCIPAL
V.P. & R.P.T.P. SCI. COLLEGE
VALLABH VIDYANAGAR-388120

V. P. & R. P. T. P. Science College

Dr. J.K. Baria
Signature of the co - Investigator
(Major Research Project)

Dr. Minal H. Patel
Signature of the Principal
Investigator
(Major Research Project)

VITTHALBHAI PATEL & RAJRATNA P. T. PATEL SCIENCE COLLEGE
VALLABH VIDYANAGAR-388 120, Dist. Anand, Guj., (India)
(Managed by Charutar Vidya Mandal)
AFFILIATED WITH SARDARPATELUNIVERSITY
Reaccredited 'A' By NAAC
Phone : (O) (02692) 230011
Cell : 9409309407
Website : www.vpscience.org.
E-mail : vprptpsc@yahoo.co.in
Dr. Bhavesh D. Patel (M.Sc., Ph. D, M.B.A(H.R.A))
PRINCIPAL

Ref. No. VRSC/2021-22/52

Date: 5th May 2021

CERTIFICATE

This is to certify that the Major Research Project titled: **Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory",** No. **F. 42-861/2013 (SR)** dated **29th October, 2014.** Awarded to **Dr. Minal H. Patel (PI)** and **Dr. J.K. Baria (CO-I),** Associate professor of Physics, has been completed and executive summary of the project has been uploaded on the college website, the URL link is

http://www.vpscience.org/materials/res project/UGC %20 MRP Dr. %20M.H.PATEL%20.pdf

http://www.vpscience.org/materials/res_project/UGC%20_MRP_Dr. %20M.H.Patel%20.PDF

This certificate is as per the requirement under prescribed Major Research Project guidelines.

Dr. Bhavesh Patel
Principal,
V. P. & R. P. T. P. Science College,
Vallabh Vidyanagar – 388 120

PRINCIPAL
V. P. & R. P. T. P. SC. COLLEGE
VALLABH VIDYANAGAR-388 120

V. P. & R. P. T. P. Science College V. V. Nagar 388120

UCO BANK

COUNTER FOIL

Form NEFT ☐ RTGS ☑

Branch V.V. Nagar

Date 23/4/2021 Time

By Cash/Cheque/Transfer for RTGS/
NEFT remittance favouring Secretary
UGC, New Delhi

Beneficiary A/c No: 8627010021222

Bank: CANARA BANK

Branch: UGC office New Delhi

IFS Code: CNRB0008627

Account Type: Savings

Amount ₹: 602258/-

Charges ₹:

Total Amount ₹:

Total Amount in words:

V.P. & R.P.T.P. Science College
Vallabh Vidyanagar 388120

Remitter Name:

Remitter A/c No: 03600200040250

Address: Vallabh Vidyanagar

FN0.42-861/2013(SR)
DR MINAL H. PATEL

Signature of Customer/Remitter

Mobile No. 9409309407

(Refer terms of remittance overleaf)

UCBAR52021042300091095

Branch Seal

V.P. & R.P.T.P. Science College V. V. Nagar 388120

Signature of Authorised Signatory

NAGAR

FD Diary No. 5589
Dated : 05-09-2014

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI 110002

F.No.42-861/2013(SR)

29 OCT 2014

The Under Secretary (FD-III)
University Grants Commission
Bahadur Shah Zafar Marg
New Delhi – 110002

Sub: **Release of Grant-in aid to Vithalbhi Patel and Rajrathan, P. T . Patel Science College, Vallabh Vidyanagar-388120 (Gujarat) for the year 2013-14 under plan in respect of Major Research Project entitled "Theoretical ..... theory" awarded to Dr. M. H. Patel, Dept. of Physics, tenure of the project from 01.4. 2013 to 31.03.2016.**

Sir,

I am directed to convey the sanction of the University Grants Commission for payment of grant of Rs.**8,35,300/- (Rupees Eight lakh Thirty Five thousand Three Hundred only)** as 1st **installment** for the year 2013-14 towards Major Research Project to **The Principal, Vithalbhi Patel and Rajrathan, P. T. Patel Science College, Vallabh Vidyanagar-388120 (Gujarat)** for the plan expenditure to be incurred during 2014-15.

Name of the Item	Amount Allocated	Head of Account	Grant now Being Sanctioned	Grant already Released	Total Grant
Book & Journals	60,000/-	3(A)2202.03.102.10.01.35	60,000/-	.....	60,000/-
Equipment	4,00,000/-		4,00,000/-	.....	4,00,000/-
Honorarium to Retd. Teacher	.....	3(A)2202.03.102.10.01.31	.....	.....	.....
Project Fellow	5,28,000/-		2,64,000/-	.....	2,64,000/-
Travel/ Fieldwork	45,000/-		22,500/-	.....	22,500/-
Chemicals	.....		.....	.....	.....
Contingency	60,000/-		30,000/-	.....	30,000/-
Hiring Services	.....		.....	.....	.....
Overhead Charges	58,800/-		58,800/-	.....	58,800/-
Additional grant	.....		.....	.....	.....
Total	11,51,800/-		8,35,300/-	.....	8,35,800/-

11. The University / Institution shall fully implement the Official Language Policy of Union Government and comply with the Official Language Act, 1963 and Official Languages (Use for Official Purposes of the Union) Rules, 1976 etc.
12. The sanction is issued in exercise of the delegation of powers vide UGC Order No. 130/2013 [F.No.10-11/12 (Admen. IA & B)] dated 28/5/2013.
13. The University / Institution shall strictly follow the UGC Regulations on curbing the menace of Ragging in Higher Education Institutions, 2009.
14. The University / Institution shall take immediate action for its accreditation by National Assessment & Accreditation Council (NAAC).
15. The accounts of the University / Institution will be open for audit by the Comptroller & Auditor General of India in accordance with the provisions of General Financial Rules, 2005.
16. The annual accounts i.e. balance sheet, income and expenditure statement and statement of receipts and payments are to be prepared strictly in accordance with the Uniform Format of Accounting prescribed by Government.
17. An amount of **Rs.....** out the grant of **Rs .....** sanctioned vide letter No. **42-861/2013(SR)dated...** has been utilized by University/College/Institution for the purpose for which it was sanctioned. Utilization Certificate for **Rs .....**has already been entered at S. NO..... Now we may enter Utilization Certificate for **Rs.....** S. No 29 and in the U.C. Registrar at page No 29.....
18. Funds to the extent of Rs..... are available under the scheme or BE / RE of the year.
19. This issues with the concurrence of IFD vide Diary No **2871**. dated **6-09-2013**
20. This issues with the approval of **Deputy** Secretary (MRP) vide Diary No.**5807** dated **11/12/2013 as revalidated by Chairman UGC for the financial Year 2014-2015 Vide Diary No. 28796 dated 7-05-2014**

Yours faithfully,

(G.S. Aulakh)
UNDER SECRETARY

Copy forwarded for information and necessary action for :-

1. **The Principal, Vithalbhi Patel and Rajrathan, P. T. Patel Science College, Vallabh Vidyanagar-388120**
2. Office of the Director General of Audit, Central Revenues, AGCR Building, I.P. Estate, New Delhi.
3. Accountant General, State Govt. of **Gujarat, Ahmadabad**
4. **Dr. M. H. Patel Deptt,of Physics, Vithalbhi Patel and Rajrathan, P. T. Patel Science College, Vallabh Vidyanagar-388120**
5. **The Registrar, Sardar Patel University, Vallabh Vidyangar**
6. Guard file.

(A.K. SINHA)
SECTION OFFICER

3

केनरा बैंक Canara Bank

U G C BRANCH, BAHADUR SHAH ZAFAR MARG, NEW DELHI – 110 002,
Telephone No: 011-23236939; 23217129 ; e-mail – cb8627@canarabank.com

REF NO: F-F-1 (FD-3) 2014
Date :06/12/2014

1954

TO
THE PRINCIPAL
VITHALBHI PATEL AND RAJRATHAN
P T PATEL SCIENCE COLLEGE
VALLABH VIDYANAGAR
388120
Sir,

I am directed to forward herewith the details of Remittances credited to your SB/CA account through **RTGS/NEFT** details of which are given below:

SENDER'S BANK		CANARA BANK, UGC, NEW DELHI
RTGS/NEFT NUMBER		CNRBR52014120600570150
DATE		06/12/2014
AMOUNT		835300/-
BENEFICIARY'S	BANK	S B I
	ACCOUNT NUMBER	31673343260
	IFSC CODE	SBIN0003119
SANCTION REFERENCE		F NO 42-861/2013(SR) F D DY 5589 DTD 05/09/2014
PURPOSE		Major research project of Dr M H Patel deptt physics

Kindly acknowledge the receipt, duly mentioning our reference.

Yours faithfully,

Manager

CC to: _____ UGC for information
Computer generated signature Not required.

UNIVERSITY GRANT COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI 110002

NAME OF THE SECTION : **SR**
Grant-in aid-Bill

1	Name of the Beneficiary Institution (University/ College/ Institute)	**Vithalbhi Patel and Rajrathan, P. T. Patel Science College, Vallabh Vidyanagar-388120**
2	Sanction No. and Date	**F.N. 42-861/2013(SR) F. D. Dy. No 5589 Dated: 05-09-2014**
3	Amount being Released	**(a)Sanctioned : Rs. 8,35,300/- (b) Adjusted: Rs. Nil (c) Net Release: 8,35,300/- (Rupees Eight lakh Thirty Five Thousand Three Hundred Only)**
4	Purpose of grant-in-aid	**Major Research Project of Dr. M. H. Patel Deptt. Physics**
5	Head of Account	**3(A)2202.03.102.10.01.31 Rs. 4,60,000/- 3(A)2202.03.102.10.01.35 Rs. 3,75,300/-**
6	Designation and address of the Authorized Officer	**The Principal, Vithalbhi Patel and Rajrathan, P. T. Patel Science College, Vallabh Vidyanagar-388120**
7	Payment Details	
(a)	Bank Name & Address of Branch	**State Bank of India, Vithal Udyognagar-388121 Dist. Anand, (Gujarat)**
(b)	Account No	**31673343260**
(c)	Type of Account : SB /Current /Cash Credit	**Current**
(d)	IFSC Code	**SBIN0003119**
(e)	MICR Code	**388002002**
f)	Whether Bank Branch is RTGS or NEFT enabled : RTGS / NEFT /Both	**Yes**
(g)	Name & Address of Account Holder	**The Principal, Vithalbhi Patel and Rajrathan, P. T. Patel Science College, Vallabh Vidyanagar-388120**

Received a sum of Rs. **8,35,300/- Rs. (Eight lakh Thirty five thousand Three Hundred Only)** being amount sanctioned vide sanction letter No. F.-No. **42-861/2013(SR)** dated 29/10/14 (copy enclosed) for disbursement to **The Principal, Vithalbhi Patel and Rajrathan, P. T. Patel Science College Vallabh Vidyanagar-388120**

Certified that the co ion of the grant has been accepted by the grantee Necessary entries in IA /Budget Control Register have been made.

(G.S. AULAKH)
UNDER SECRETARY

23236351, 23232701, 23237721, 23234116

विश्वविद्यालय अनुदान आयोग
बहादुरशाह जफर मार्ग
नई दिल्ली-110 002
UNIVERSITY GRANTS COMMISSION
BAHADURSHAH ZAFAR MARG
NEW DELHI-110 002

SPEED POST

14 DEC 2014

F.No. 42-861/2013(SR)

November, 2014

Dr. M.H. Patel
Deptt. of Physics,
Vitthalbhai Patel and Rajrathan, P.T.Patel Science College
Vallabh Vidyanagar

Sub:-**Major Research Project-Midterm Evaluation**.

Sir/Madam,

This has reference to the Major Research Project awarded to you by the University Grants Commission.

As per the guidelines of the scheme, the progress of the work done on the project is to be evaluated by the UGC with the help of Mid-term Expert Committee. Accordingly, the UGC has organised Mid-term Review Expert Committee meeting in the subject of **Physics** on **12.01.2015** at 10.00 AM in the UGC Office at Bahadur Shah Zafar Marg, New Delhi-110 002 (Details on ugc website www.ugc.ac.in). The evaluation will be carried out in the form of discussion/presentation with the Expert Committee.

You are requested to bring three copies of downloaded application duly filled in with details of progress of research work forwarded through the Registrar/Principal only alongwith the details of Project Fellow in the prescribed proforma (Annexure-VI) as per XII Plan guidelines of Major Research Project.

It is mandatory that Principal Investigator only should attend the above Mid-term Review Expert Committee meeting. The expenditure on travel by Principal Investigator could be met out of the project fund as per your entitlement in your Institution. If the Principal Investigator fails to attend the meeting, the UGC may consider to withdraw the project/stop further support for the project. The recommendations of the UGC Mid-term Review Expert Committee would decide the continuance/discontinuance of the project.

Yours faithfully,

Nidhi Sharma

(DR.NIDHI SHARMA)
DEPUTY SECRETARY

Encls:As above

PROFORMA FOR SUPPLYING THE INFORMATION IN RESPECT OF THE STAFF APPOINTED UNDER THE SCHEME OF MAJOR RESEARCH PROJECT

UGC FILE NO. F._____(SR/MRP) YEAR OF COMMENCEMENT ☐☐ ☐☐ ☐☐☐☐

TITLE OF THE PROJECT :

1.	Name Of the Principal Investigator :	Prof./Dr.
2.	Name of the University/College	
3.	Name of the Research Personnel appointed	
4.	Academic qualification	S.No. / Qualifications / Year / Marks / %age 1. M.A./M.Sc./M.Tech. 2. M.Phil 3. Ph.D.
5.	Date of joining	
6.	Date of Birth of Research Personnel	
7.	Amount of HRA, if drawn	
8.	Number of Candidate applied for the post	

CERTIFICATE

This is to certify that all the rules and regulations of UGC Major Research Project outlined in the guidelines have been followed. Any lapse on the part of the University will liable to terminate of said UGC project.

Principal Investigator | Head of the Deptt. | Registrar/Principal

From: Dr. Minal H. Patel
Associate Professor in Physics,
V. P. & R. P. T. P. Science College,
Vallabh Vidhyanagar – 388 120
8th January 2015

To,
The Secretary,
UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002

Sub: Submission of the mid-term evaluation report of my Major Research Project...

Dear Sir,

We have received the Major Research Project from University Grants Commission (UGC) New Delhi, entitled **"Theoretical investigation of transition metal and their alloys using ab-initio pseudopotential theory"** vide letter **No. F. 42-861/2013 (SR)** dated **29th October 2014**. The grant of this project has been credited to our account in the month of December 2014. So, all the process of purchasing of equipment and appointment of JRF is under progress. Hence, the project work is not executed. So we request you to extend the tenure of our Major Research Project from January-2015 to December-2018.

Thanking You,

Signature of the Principal
With seal of the college
PRINCIPAL
V. P. & R. P. T. P. SCI. COLLEGE
VALLABH VIDYANAGAR-388120

V.P. & R.P.T.P. Science College V. V. Nagar 388120

Signature of the Principal
Investigator
(Major Research Project)

Signature of the Principal
Co-Investigator
(Major Research Project)

विश्वविद्यालय अनुदान आयोग
University Grants Commission
मानव संसाधन विकास मंत्रालय, भारत सरकार
(Ministry of Human Resource Development, Govt. of India)
बहादुरशाह जफर मार्ग नई दिल्ली –110002
Bahadurshah Zafar Marg, New Delhi-110002

सत्यमेव जयते

ज्ञान-विज्ञान विमुक्तये

No. F. 42-861/2013 (SR)

March, 2016 APR 2016

The Principal,
Vitthalbhai Patel and Rajrathan,
P.T. Patel College, Vallabh
Vidyanagar, Anand, Gujarat-388120.

Subject:- Extension of Major Research Project awarded **Dr. M.H. Patel , Department of Physics** by UGC during 2013.

Sir,/ Madam,

I am directed to say that the tenure of the Major Research Project awarded to you has been extended by the UGC upto 31.03.2017 without any financial assistance for the extended period.

Yours faithfully,

(G. S. Aulakh)
Under Secretary

To, M H. Patel

2/4

2/4

Annexure - III

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002

STATEMENT OF EXPENDITURE IN RESPECT OF MAJOR RESEARCH PROJECT

1. Name of Principal Investigator : **Dr. Minal H. Patel, [Name of the Co – Investigator: Dr. J.K. Baria]**
2. Deptt. of Principal Investigator : **Physics**
University/College **VP & RPTP Science College, Vallabh Vidyanagar 388 120**
3. UGC approval Letter No. and Date : **F. 42-861/3 (SR)** dated **29th October 2014**
4. Title of the Research Project : **"Theoretical investigation of transition metal and, their alloys using ab- initio pseudopotential theory"**
5. Effective date of starting the project **29th October 2014**
6. a. Period of Expenditure: From **29th October, 2014** to **May, 2021**
b. Details of Expenditure

S.No.		Item	Amount Approved (Rs.)	1st Instalment	Expenditure Incurred (Rs.)	Balance Amount
i.	Non-recurring	Books & Journals	60,000/-	4,60,000/-	36,340/-	-23,660/-
ii.		Equipment	4,00,000/-		1,23,590/-	-2,76,410/-
iii.	Recurring	Contingency	60,000/-	3,75,300/-	475/-	-29,525/-
iv.		Field Work/Travel (Give details in the proforma at Annexure-IV).	45,000/-		13,837/-	-8,663/-
v.		Hiring Services	-		-	-
vi.		Chemicals & Glassware	-		-	-
vii.		Overhead	58,800/-		58,800/-	NIL
viii.		Any other items (Please specify) honorarium to Project Fellow	5,28,000/-			-2,64,000/- (Project fellow not appointed)
		Total	11,51,800/-	8,35,300/-	2,33,042 /-	-6,02,258/-

c . Staff
Date of Appointment : **Not Appointed**

S.No	Items	From	To	Amount Approved (Rs.)	Expenditure incurred (Rs.)
1.	Honorarium to PI (Retired Teachers) @ Rs. 18,000/-p.m.	-	-	**2,64,000/-**	-
2.	**Project fellow:** i) **NET/GATE qualified**-Rs. 16,000/- p.m. for initial 2 years and Rs. 18,000/- p.m. for the third year. ii) **Non-GATE/Non-NET**- Rs. 14,000/- p.m. for initial 2 years and Rs. 16,000/- p.m. for the third year.	-	-		

1. It is certified that the appointment(s) have been made in accordance with the terms and conditions laid down by the Commission.

2. If as a result of check or audit objection some irregularly is noticed at later date, action will be taken to refund, adjust or regularize the objected amounts.

3. Payment @ revised rates shall be made with arrears on the availability of additional funds.

4. It is certified that the grant of **Rs. 8,35,300/- (Rupees six lakhs eighty six thousands only)** received from the University Grants Commission under the scheme of support for Major Research Project entitled **"Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory"** vide UGC letter No. F. **F. 42-861/2013 (SR)** dated **29th October 2014,** has been partially utilized for the purpose for which it was sanctioned and in accordance with the terms and conditions laid down by the University Grants Commission.

Dr. Minal H. Patel
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. J.K. Baria
(Co-Investigator)
Associate Professor in Physics,
V P & R P T P Science college,
Vallabh Vidyanagar – 388 120

Dr. Bhavesh Patel
PRINCIPAL
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

PRINCIPAL
V.P. & R.P.T.P. SCI. COLLEGE
VALLABH VIDYANAGAR-388120

V. P. & R. P. T. P. Science College

Annexure - IV

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002

STATEMENT OF EXPENDITURE INCURRED ON FIELD WORK

Name of the Principal Investigator: Dr. Minal H. Patel

Name of the Place visited	Duration of the Visit		Mode of Journey	Expenditure Incurred (Rs.)
	From	To		
UGC New Delhi	11th January, 2015	13th January, 2015	By Train	6,907/-
UGC New Delhi	28th July, 2015	30th July, 2015	By Train	6,930/-
Total traveling expenditure				13,837/-

Certified that the above expenditure is in accordance with the UGC norms for Major Research Project.

Dr. Minal H. Patel
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. J.K. Baria
(Co-Investigator)
Associate Professor in Physics,
V P & R P T P Science college,
Vallabh Vidyanagar – 388 120

Dr. Bhavesh Patel
PRINCIPAL
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

PRINCIPAL
V.P. & R.P.T.P. SCI. COLLEGE
VALLABH VIDYANAGAR-388120

V. P. & R. P. T. P. Science College V. V. Nagar 388 120

Annexure – V

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002.

Utilization Certificate

Certified that the grant of Rs. **8,35,300.00** (Rupees **Eight lakhs thirty five thousand and three hundred only**) received from the University Grants Commission under the scheme of support for Major Research Project entitled **"Theoretical investigation of transition metal and their alloys using ab-initio pseudopotential theory"** vide UGC letter **No. F. 42-861/2013 (SR)** dated **29th October 2014** has been partially utilized (separate statement of bifurcation is shown in **appendix-A**) for the purpose for which it was sanction and in accordance with the terms and conditions laid down by the University Grants Commission. We have utilised Rs. **2,33,042/-** (rupees Two lakhs thirty-three thousand forty-two) and remaining balance of Rs. **6,02,258/-** (Rupees Six lakhs two thousand two hundred fifty -eight).

Apaji Amin & Co. LLP
Chartered Accountants
Firm Regn. No. 100513W/W100062

Dr. Bhavesh Patel
Signature of the Principal
With seal of the college

Dr. Minal H. Patel
Signature of the Principal Investigator
(Major Research Project)

Dr. J.K. Baria
Signature of the Co Investigator
(Major Research Project)

Tehmul B. Sethna
Partner, M.No. 035476
Signature of the Chartered Accountant
With Registration number and seal

Udin: 21035476AAAACKR2467

Appendix - A

Financial Assistance Provided/Expenditure incurred:

S.No.		Item	Amount Approved (Rs.)	1st Instalment	Expenditure Incurred (Rs.)	Balance Amount
i.	Non-recurring	Books & Journals	60,000/-	4,60,000/-	36,340/-	-23,660/-
ii.		Equipment	4,00,000/-		1,23,590/-	-2,76,410/-
iii.	Recurring	Contingency	60,000/-	30,000/-	475/-	-29,525/-
iv.		Field Work/Travel (Give details in the proforma at Annexure- IV).	45,000/-	22,500/-	13,837/-	-8,663/-
v.		Hiring Services	-		-	-
vi.		Chemicals & Glassware	-		-	-
vii.		Overhead	58,800/-	58.800/-	58,800/-	NIL
viii.		Any other items (Please specify) honorarium to Project Fellow	5,28,000/-	2,64,000/-	-	-2,64,000/- (Project fellow not appointed)
		Total	11,51,800/-	8,35,300/-	2,33,042 /-	-6,02,258/-

It is certified that the grant of Rs **8,35,300.00** (Rupees **Eight lakhs thirty five thousand and three hundred only**) received from the University Grants Commission under the Scheme of support for Major Research Project entitled **"Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory"** vide UGC Letter **No. F. 42-861/2013 (SR)** dated **29th October 2014** has been partially utilized for the purpose for which it was sanctioned and in accordance with the terms and conditions laid down by the University Grants Commission . We have utilised Rs. **2,33,042/-** (rupees Two lakhs thirty-three thousand forty-two) and remaining balance of Rs. **6,02,258/-** (Rupees Six lakhs two thousand two hundred fifty -eight).

Dr. Bhavesh Patel
Signature of the Principal
With seal of the college

Dr. Minal H. Patel
Signature of the Principal Investigator
(Major Research Project)

Dr. J.K. Baria
Signature of the Co-Investigator
(Major Research Project)

Apaji Amin & Co. LLP
Chartered Accountants
Firm Regn. No. 100513W/W100062

Tahmul B. Vakharia
Partner, M.No. 038478

Signature of the Chartered Accountant
With Registration number and seal

UDIN: 21038478AAAACR2469

Annexure – V

ज्ञान-विज्ञान विमुक्तये

Annexure - VI

PROFORMA FOR SUPPLYING THE INFORMATION IN RESPECT OF THE STAFF APPOINTED UNDER THE SCHEME OF MAJOR RESEARCH PROJECT

UGC File No. F. 42-861/2013 (SR) dated: **29th October 2014**

Title of the Project: "entitled **"Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory"**

1.	Name of the principal investigator Name of the co – investigator	**Dr. Minal H. Patel** **Dr. J.K. Baria**				
2.	Name of the College/University	**VP & RPTP Science College, Vallabh Vidyanagar** **Sardar Patel University, Vallabh Vidyanagar**				
3.	Name of the research Personnel appointed.	**Not appointed**				
4.	Academic qualification	**Sr. No.**	**Qualification**	**Year**	**Marks**	**%**
		-	-	-	-	-
5.	Date of Joining	-				
6.	Date of birth of research Personnel	-				
7.	Amount of HRA, if drawn	-				
8.	Number of candidate applied for the post	**Nil**				

Certificate

This is to certify that all the rules and regulations of UGC Major Research Project outline in the guidelines have been followed. Any lapses on the part of the University will liable to terminate of said UGC project.

Dr. Minal H. Patel
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. J.K. Baria
(Co-Investigator)
Associate Professor in Physics,
V P & R P T P Science college,
Vallabh Vidyanagar – 388 120

Dr. Bhavesh Patel
PRINCIPAL
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

PRINCIPAL
V.P. & R.P.T.P. SCI. COLLEGE
VALLABH VIDYANAGAR-388120

V. P. & R. P. T. P. Science College

Annexure – VII

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002

MAJOR RESEARCH PROJECT COPY OF THE SPECIMEN OF HOUSE RENT FOR PROJECT FELLOW

Certified that Shri/Dr._____NA_____ is paying House Rent of Rs. _____-_____ and is eligible to draw House Rent Allowances @_____-_____ as per University Rules.

Registrar/Principal
(Signature with Seal)

Certified that Shri/Dr. _____NA_____ is not staying independently and therefore is eligible to draw House Rent @ of Rs. _____-_____p.m. minimum admissible to a Lecturer as per University Rules.

Registrar/Principal
(Signature with Seal)

Certified that Shri/Dr. _____NA_____ has been provided accommodation in the Hostel. But he/she could not be provided with single seated flat type accommodation as recommended by the Commission, Hostel fee @ Rs._____-_____ per month w.e.f. _____-_____ is being charged from him/her.

Dr. Minal H. patel
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. J.K. Baria
(Co-Investigator)
Associate Professor in Physics,
V P & R P T P Science college,
Vallabh Vidyanagar – 388 120

Dr. Bhavesh Patel
PRINCIPAL
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

PRINCIPAL
V.P. & R.P.T.P. SCI. COLLEGE
VALLABH VIDYANAGAR-388120

V. P. & R. P. T. P. Science College

Annexure -VIII

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002.
Final Report of the work done on the Major Research Project.
(Report to be submitted within 6 weeks after completion of each year)

Final Report

1. Project report.:
2. UGC Reference No.F. **F. 42-861/2013 (SR)** dated **29th October 2014**
3. Period of report: from **29th October, 2014 to May, 2021**
4. Title of research project **"Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory"**
5. (a) Name of the Principal Investigator/ Co Investigator: **Dr. Minal H. Patel/Dr. J.K. Baria**
   (b) Deptt. : Physics, **VP & RPTP Science College, Vallabh Vidyanagar**
   (c) University/College where work has progressed **VP & RPTP Science College, Vallabh Vidyanagar.**
6. Effective date of starting of the project: **29th October, 2014**
7. Grant approved and expenditure incurred during the period of the report:

a. Total amount approved Rs. **8,35,300/-**
b. Total expenditure Rs. **2,33,042/-**
c. Report of the work done: (Please attach a separate sheet)
i. Brief objective of the project: **results achieved**
ii. Work done so far and results achieved and publications, if any, resulting from the work (Give details of the papers and names of the journals in which it has been published or accepted for publication **04**
iii. Has the progress been according to original plan of work and towards achieving the objective. if not, state reasons: **Yes, According to plan**
iv. Please indicate the difficulties, if any, experienced in implementing the project: **yes, we did not get Wein2k software**
v. If project has not been completed, please indicate the approximate time by which it is likely to be completed. A summary of the work done for the period (Annual basis) may please be sent to the Commission on a separate sheet.
vi. If the project has been completed, please enclose a summary of the findings of the study. One bound copy of the final report of work done may also be sent to University Grants Commission.
vii. Any other information which would help in evaluation of work done on the project. At the completion of the project, the first report should indicate the output, such as (a) Manpower trained (b) Ph. D. awarded (c) Publication of results (d) other impact, if any

Dr. Minal H. Patel
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. J.K. Baria
(Co-Investigator)
Associate Professor in Physics,
V P & R P T P Science college,
Vallabh Vidyanagar – 388 120

Dr. Bhavesh Patel
PRINCIPAL
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

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V. P. & R. P. T. P. Science College • V. V. Nagar 388 120

Library Accession Certificate

This is to certify that the following books are purchased by Dr. M. H. Patel during his UGC MAJOR RESEARCH PROJECT entitled **"Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory"** [Grant No. **F. 42-861/2013 (SR)** dated **29th July 2014**] and these books are submitted in the college library.

Dr.L. M. Katara
Librarian
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

V.P. & R.P.T.P. Science College * LIBRARY * V. V. Nagar

Dr. Minal H. Patel
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. J.K. Baria
(Co-Investigator)
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. Bhavesh Patel
PRINCIPAL
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

PRINCIPAL
V.P. & R.P.T.P. SCI. COLLEGE
VALLABH VIDYANAGAR-388120

V. P. & R. P. T. P. Science College

Sr No	Title of the book	Author(s)	Publisher	Library accession number
1	Condensed Matter Physics	Bal Krishna Agrawal	Narosa Publishing House	50542
2	Quantum Mechanics	B. H. Bransden	Pearson Education	50543
3	Introductory Statistical Mechanics	Roger Bowley	Oxford University Press	50544
4	Mathematical Methods for Physics and Engineering	K. F. Riley	Cambridge University Press	50545
5	Equilibrium Thermodynamics,3rd edition	C.J. Adkins	Cambridge University Press	50546
6	Problems in Quantum Mechanics with solutions	G.L. Squires	Cambridge University Press	50547
5	The Art of Molecular Dynamic Simulation	D. C. Rapaport	Cambridge University Press	50548
6	Electronic Structure and Properties of	Isaac B. Bersuker	John Wiley India Pvt. Ltd.	50549
7	Electronic Structure of Materials	Rajendra Prasad	CRC Press	50551
8	Eintein:His Life and Universe	Walter Isaacson	Pocket Books	50558
9	The Innovators	Walter Isaacson	Pocket Books	50559
10	The Turning Point	Capra	Flaminge	50560
11	The TAO of Physics	Capra	Flaminge	50561
12	Uncommon Wisdom	Capra	Flaminge	50562
13	The Theory of Every Thing	Stephen W. Hawking	Jaico Publication	50563
14	Nanosicence and Nanotechnology :Fundamentals to Frontiers	M. S. Ramachandra Rao	Wiley India Pvt. Ltd.	50564
15	Introduction to Special Relativity	Robert Resnik	Wiley India Pvt. Ltd.	50565
16	Nanotechnology:Importance and Application	M. H. Fulekar	I. K. International Publishing	50566
17	Nanotechnology:Fundamentals and Applications	Mansi Karkare	I. K. International Publishing	50567
18	An Introductory Course of Statistical Mechanics	Palash B. Pal	Narosa Publishing House	50568
19	An Introduction to Energy Conversion:Turbomachinery	Kadambi Prashad	New Age International Publishers	50569
20	Problems and Solutions on Thermodynamics and statistical Mechanics	Yung Kuo Lim	Sarat Book House	50570
21	Introduction to Nanoscience and Nanotechnology	K. K. Chattopadhyay	PHI Learning Pvt. Ltd.	50571

Dr.L. M. Katara
Librarian
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

V. P. & R. P. T. P. Science College LIBRARY V. V. Nagar

Dr. Minal H. Patel
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. J.K. Baria
(Co-Investigator)
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. Bhavesh Patel
PRINCIPAL
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

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Assets Certificate

I have submitted the completion report on UGC MAJOR RESEARCH PROJECT entitled "**Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory**" [Grant No. **F. 42-861/2013 (SR)** dated **29th October 2014**] and necessary document to UGC on, May, 2021. I have purchased following items during the project

1. Desktop Lenovo All in One A740 F0AM004MIN batch :LIN240315

   Intel cire i7 4558U(2.8Ghz),H 81, 8GB DDR3, 1TB+8GBssHD, wireless, 1080P

   2GB Nvidia GT840A, HDMI,27" 10 point

   Touch LED, Win 8.1SL64 Bit

2. Laser printer [HP canon-3010 B]

3. UPS 1 KVA Power safe

I am submitting these items to the college.

Dr. Minal H. Patel
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. J. K. Baria
(Co-Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. Bhavesh Patel
PRINCIPAL
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

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Annexure - IX

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI - 110 002

PROFORMA FOR SUBMISSION OF INFORMATION AT THE TIME OF SENDING THE FINAL REPORT OF THE WORK DONE ON THE PROJECT

1. Title of the Project : **"Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory"**
2. NAME AND ADDRESS OF THE PRINCIPAL INVESTIGATORCo Investigator: **Dr. Minal H. Patel/ Dr. J.K. Baria**
3. NAME AND ADDRESS OF THE INSTITUTION **VP & RPTP Science College, Vallabh Vidhyanagar 388 120**
4. UGC APPROVAL LETTER NO. AND DATE **F. 42-861/2013 (SR)** dated **29th October 2014**
5. DATE OF IMPLEMENTATION : **29th October, 2014**
6. TENURE OF THE PROJECT : **three years**
7. TOTAL GRANT ALLOCATED : **11,51,800/-**
8. TOTAL GRANT RECEIVED : **8,35,300/-**
9. FINAL EXPENDITURE : **2,33,042/-**
10. TITLE OF THE PROJECT **"Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory"**
11. OBJECTIVES OF THE PROJECT : **Achieved**

- To construct model potentials and used in the present investigation.
- To explore the use of model potential in the study of various physical properties in the ordered and disordered form of
  - Noble metals
  - Transition metals
  - Compounds and alloys of these metals and elements
- To carry out the theoretical investigations of various physical properties using molecular dynamics (**MD**), at the latter stage we may use Monte Carlo simulation methods and ab-initio method to calculate the same physical properties.
- To predict the usefulness of pseudopotential theory in the study of binary alloys and metallic glass.
- To investigate the impact of various exchange and correlation functions in the aforesaid study.

12. WHETHER OBJECTIVES WERE ACHIEVED
Yes, it was achieved and briefly discussed in work done.

13. ACHIEVEMENTS FROM THE PROJECT:
We have calculated structure dependent properties of liquid metals at various temperatures such as Dynamical elastic constants, Velocity autocorrelation function, Diffusion

coefficient, Phonon dispersion curves, Characteristic frequency, Power spectrum, Viscosity and Surface tension of these metals their compound and alloys.

14. SUMMARY OF THE FINDINGS: **See Appendix-B**
15. CONTRIBUTION TO THE SOCIETY:
The research which has been carried out will be helpful to the future researchers for extend their research further.
16. WHETHER ANY PH.D. ENROLLED/PRODUCED OUT OF THE PROJECT: **No**
17. NO. OF PUBLICATIONS OUT OF THE PROJECT: **04**
(PLEASE ATTACH)

Dr. Minal H. Patel
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

Dr. J.K. Baria
(Co-Investigator)
Associate Professor in Physics,
V P & R P T P Science college,
Vallabh Vidyanagar – 388 120

Dr. Bhavesh Patel
PRINCIPAL
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

PRINCIPAL
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VALLABH VIDYANAGAR-388120

V. P. & R. P. T. P. Science College

Annexure – X

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002

ASSESSMENT CERTIFICATE

(to be submitted with the proposal)

It is certified that the proposal entitled **"Theoretical investigation of transition metal and their alloys using ab - initio pseudopotential theory"** vide UGC letter **No. F. 42-861/2013 (SR)** dated **29thOctober 2014.** By (Dr./Prof./Mr./Mrs.)**Dr.Minal H. Patel(P.I) &Dr. J. K. BARIA (CO-I.)Deptt. Of Physics, VP & RPTP Science College, Vallabh Vidyanagar** has been assessed by the **Two members**committee consisting the following members for submission to the University Grants Commission, New Delhi for financial support under the scheme of Major Research Projects:

Details of Expert Committee:

	Name of Expert	Name of Department	Signature with Date
1	Prof. N. K. Bhatt	Professor of Physics, Department of Physics, M. K. Bhavnagar University, Bhavnagar – 364001 Gujarat	01/05/2021
2	Prof. Pankajsinh Thakor	Professor of Physics, Department of Physics, Veer Narmad South Gujarat University, Gujarat	01/05/2021

The proposal is as per the guidelines.

(REGISTRAR/ PRINCIPAL)
(Seal)

PRINCIPAL
V. P. & R. P. T. P. SC. COLLEGE
VALLABH VIDYANAGAR-388 120

V.P. & R.P.T.P. Science College V.V. Nagar 388120

Annexure – XI

Final Report Assessment / Evaluation Certificate
(Two Members Expert Committee Not Belonging to the Institute of Principal Investigator)
(to be submitted with the final report)

It is certified that the final report of Major Research Project entitled "**Theoretical investigation of transition metal and their alloys using ab- initio pseudopotential theory**" vide UGC letter **No. F. 42-861/2013 (SR)** dated **29thOctober 2014.** By (Dr./Prof./Mr./Mrs.)**Dr.Minal H. Patel(P.I) &Dr. J. K. BARIA (CO-I.)**Deptt. Of **Physics, VP & RPTP Science College, Vallabh Vidyanagar** has been assessed by the **Two members**committee consisting the following members for final submission of the report to the UGC, New Delhi under the scheme of Major Research Project.

Comments/Suggestions of the Expert Committee:

The major objectives set in the Research Proposal as referenced above were met. In particular, the structural information like pair-correlation function and structure factors generated for noble metal silver using molecular dynamics simulations, and crystal and heat solvation energies for some solid solutions were reported. The author(s) purchased a computing system to perform these calculations. In lieu of *project fellow*, the outcome of the project seems satisfactory, and can be considered for its closer procedure.

Name & Signatures of Experts with Date:-

	Name of Expert	University/College name	Signature with Date
1	Prof. N. K. Bhatt	Professor of Physics, Department of Physics, M. K. Bhavnagar University, Bhavnagar – 364001 Gujarat	01/05/2021
2	Prof. Pankajsinh Thakor	Professor of Physics, Department of Physics, Veer Narmad South Gujarat University, Gujarat	01/05/2021

It is certified that the final report has been uploaded on UGC-MRP portal on 2021.
It is also certified that final report, Executive summary of the report, Research documents, monograph, academic papers provided under Major Research Project have been posted on the website of the University/College.

(Registrar/Principal)
Seal

PRINCIPAL
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V. P. & R. P. T. P. Science College
V. V. Nagar 388120

APPENDIX – C

Dr. Minal H. Patel

Papers presented in the conferences:

1. Computational Study of Total Crystal energy and Heat of solution of Li- Na, Li – K, Li- Rb and Li – Cs solid solutions

   Minal H. Patel and P.N. Gajjar

   International conference on New Scintillations on Material Horizon (ICNSMH-2016) Proceeding October 2016

   Department of applied physics, Faculty of engineering and technology, MJPR university- BAREILLY

2. Structural Studies of Liquid Silver at various Temperatures Using Molecular Dynamics Simulation Technique

   A.R.Jivani, P.S.Vyas, Minal H. Patel and J.K. Baria

   National Conference on Recent Trends in Science of Materials (NCSM- 2K15) proceeding December 2015- M. S. University of Baroda

Dr. J.K. Baria

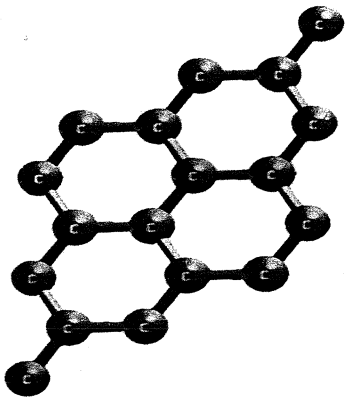
1. Refractive index of $B_{1-x}Ga_xN$ semiconductors
   P.S. Vyas, J.K. Baria, A.R. Jivani, P.N. Gajjar and A.R. Jani
   AIP conference proceedings 1536, 327(2013)
2. Elastic constants and pressure derivative of elastic constants of $Si_{1-x}Ge_x$ solid solution
   A.R. Jivani, J.K. Baria, P.S. Vyas and A.R. Jani
   AIP conference proceedings 1512, 1062 (2013)
3. LASER welding process for RF Connectors for Space Applications
   Sakaram Srinivasulu, Shivendra Tripathi, R.K. Hegde, J.K. Baria
   International journal of Emerging Technology and advanced Engineering

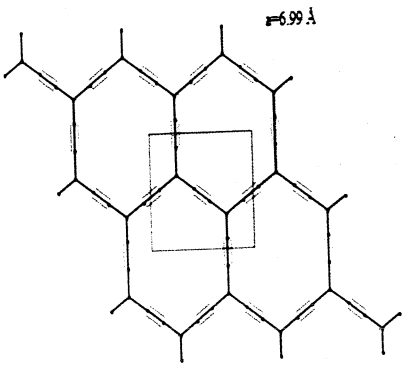
National Conference on Recent Trends in Science of Materials (NCSM - 2K15)

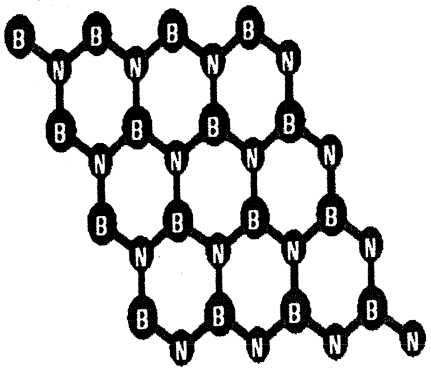
28 – 30 December, 2015

Faculty of Science,
The M. S. University of Baroda,
Vadodara

Abstracts







Sponsored By :

DST-PUSRE and UGC Merged Programmes

Structural Studies of Liquid Silver at Various Temperatures Using Molecular Dynamics Simulation Technique

A. R. Jivani, P. S. Vyas, Minal H. Patel and J. K. Baria,

V. P. & R. P. T. P. Science College, Vallabh Vidyanagar – 388 120, Gujarat, India
Email: jay_baria@yahoo.com

Abstract. Molecular Dynamics (MD) simulation techniques has been used for the investigation of pair distribution function g(r), and structure factor S(q) of liquid Silver at various temperature with pseudopotential proposed by us. Good agreement with the experiment values are observed for the pair distribution function, and structure factor. The present investigations are also compared with the results obtained by other theoretical calculations, showing the transferability of the pseudopotential used from solid to liquid environment in the case of silver.

Keywords: **Molecular dynamics, pair distribution function, structure factor, coordination number.**

International Conference on New Scintillations on Materials Horizon (ICNSMH-2016)

21-23 OCTOBER, 2016

Souvenir & Abstracts

Organized By

Department of Applied Physics

Faculty of Engineering and Technology

MAHATMA JYOTIBA PHULE ROHILKHAND UNIVERSITY

BAREILLY, INDIA

Sponsored by TEQIP-I, MHRD, New Delhi

ICNSMH-2016

with solubilization of metals and hydrolysis of other chemical compounds. The present study reports the CNT sensitivity for hydrogen flouride (HF) in its pristine as well as edge decorated one, by analysing its electronic properties in terms of band structure and conductance measures through two probe model in vacuum as well as HF gas environment. The hydrogen fluoride sensing ability of pristine as well as Si decorated (10,0) single walled carbon nanotube has been analyzed by using a DFT based ab-initio approach, applied through Generalized Gradient Approximation with Perdew, Burke and Ernzerhof type parameterization. The sensing of toxic hydrogen fluoride through nanotube has been analysed in terms of its band structure and density of state profile variation and conductance analysis. In case of pristine nanotube as shown in Fig (a), the analysis observes a band gap of about 0.7 eV, reduces to 0.4 for Si decorated carbon nanotube and further drastic fall in band gap in case of Si decorated nanotube due to presence of HF molecule near the surface. The zero bias sensitivity has been verified through conductance analysis, which verifies the observations on bandgap variation.

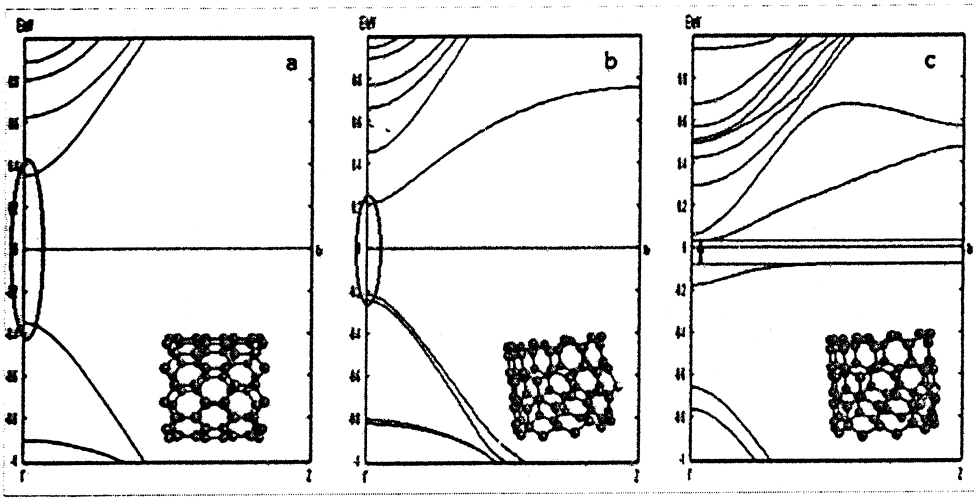


Fig: Band structure profiles of (a) pristibe (b) si-decorated and (c) HF adsorbed Si-decorated CNT

PP 31

Computational Study of Total Crystal Energy and Heat of Solution of Li-Na, Li-K, Li-Rb, and Li-Cs Solid Solutions

Minal H Patel[1] and P. N. Gajjar[2]

[1]V.P. and R. P. T. P. Science College, Vallabh Vidyanagar 388 120, Gujarat, India
[2]Department of Physics, University School of Sciences, Gujarat University, Ahmedabad 380 009, Gujarat, India
E-mail: mhp67@rediffmail.com, pngajjar@rediffmail.com

Abstract

The total crystal energy and heat of solutions of Li-Na, Li-K, Li-Rb and Li-Cs solid solutions are investigated using pseudo alloy atom model. In the present investigation our model potential is used to explain interaction. To include exchange and correlation effects, Hartree, Taylor, Ichimaru-Utsumi, Farid et al. and Sarkar-Sen local field corrections are used. It is concluded that these alloys have small and positive value of heat of solution in the entire range of concentration. It is also concluded that for Li based alloys as we go from Na to Cs, the metal having smaller in atomic size give a smaller energy differenceindicating a larger solubility. Hence Na is more soluble in Li compared to Cs.

AIP Conference Proceedings

Refractive index of B1−xGaxN semiconductors

P. S. Vyas, J. K. Baria, A. R. Jivani, P. N. Gajjar, and A. R. Jani

Citation: AIP Conf. Proc. **1536**, 327 (2013); doi: 10.1063/1.4810233
View online: http://dx.doi.org/10.1063/1.4810233
View Table of Contents: http://proceedings.aip.org/dbt/dbt.jsp?KEY=APCPCS&Volume=1536&Issue=1
Published by the AIP Publishing LLC.

Refractive Index of $B_{1-x}Ga_xN$ Semiconductors

P. S. Vyas[*], J. K. Baria[*], A. R. Jivani[*], P. N. Gajjar[#], A. R. Jani[†]

[*]*V. P. and R. P. T. P. Science College, Vallabh Vidyanagar 388 120, Gujarat, INDIA*
[†]*Department of Physics, Sardar Patel University, Vallabh Vidyanagar 388 120, Gujarat, INDIA*
[#]*Department of Physics, University School of Sciences, Gujarat University, Ahmedabad 380 009, Gujarat, INDIA*

Abstract. A theoretical procedure is presented for the study of refractive index of ternary alloy $B_{1-x}Ga_xN$. The calculations based on the pseudopotential formalism in which local potential coupled with the virtual crystal approximation (VCA) is applied to evaluate energy band gap at point X on the Jones-zone face, refractive index for the entire range of the alloy composition x of the ternary alloy $B_{1-x}Ga_xN$. To include exchange and correlation effects, local field correction function due to Nagy is employed. Our results for parent compounds are compared to experiment and other available theoretical findings and showed generally good agreement. During present study it is found that the refractive index of the ternary alloy $B_{1-x}Ga_xN$ has minimum value at gallium concentration $x = 0.4$.

Keywords: Pseudopotential; semiconductor compounds; refractive index.
PACS: 71.15Dx, 71.20.Nr, 78.20.Ci

INTRODUCTION

Recently the nitride compounds and their ternary alloys have been attracting considerable attention because of their wide range of potential applications such as air and water purification, deep ultraviolet light emitting diodes, laser diodes, optical detectors for high-frequency electronic devices, surface disinfection, ultraviolet curing and medical phototherapy. BN and GaN have wide band gap ranging from the ultraviolet to the visible regions of the spectrum, strong inter-atomic bonds, high thermal conductivity, a high melting temperature, high bulk modulus and a low dielectric constant [1], which make them to be an ideal materials for optoelectronic and high-temperature and high-power devices. Due to higher sensitivity towards external influence such as temperature, external fields and strains, these materials become strong candidates for sensors too.

The energy band gap and the refractive index of semiconductors represent two fundamental physical aspects that characterize their optical and electronic properties. The energy gap determines the threshold for absorption of photons in semiconductors and the refractive index in the semiconductor is a measure of its transparency to incident radiation. The devices such as photonic crystals, wave guides, solar cells and detectors require a pre-knowledge of the refractive index and energy gap. Many attempts have been made to correlate the energy band gap to the optical refractive index of semiconductors. In the present paper we have used novel model potential bearing a single parameter with using the improved virtual crystal approximation (VCA) [2] to study energy band gap at point X on the Jones-zone face and the composition effect on refractive index using Ravindra-Srivastava relation (RI_1) [3], Reddy-Ahammed relation (RI_2) [4] along with the basic Moss relation (RI_3) [5] of semiconductor ternary alloy $B_{1-x}Ga_xN$.

THEORY

The bare-ion potential [2] used in the present investigations is proposed in **r**-space,

$$\left.\begin{aligned} W^{ion}(r) &= -\frac{Ze^2}{2R_c}\left[2-\left(2-\frac{r}{R_c}-\frac{r^2}{R_c^2}\right)exp\left(\frac{-r}{R_c}\right)\right], && r \le R_c \\ W^{ion}(r) &= -\frac{Ze^2}{r}, && r \ge R_c \end{aligned}\right\} \quad (1)$$

With Z, e and R_c are valency, electronic charge and pseudo core radius respectively. Here R_c is estimated through zero pressure condition [6]. The local field correction function due to Nagy [7] is employed to include exchange and correlation effects.

RESULTS & DISCUSSIONS

The input parameters are given in Table 1. The energy band gap at point X on the Jones-zone face and refractive index computed by above mentioned three relations for binary compounds BN and GaN are shown in Table 2.

TABLE 1. Input Parameters

Element	Structure	Atomic Volume ($a.u^3$)
BN	zinc-blende	39.88
GaN	zinc-blende	76.90

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TABLE 2. Energy band gap (eV) and refractive index (RI) for BN and GaN

Property	BN			GaN		
	Cal.	Expt.	Others	Cal.	Expt.	Others
$E_g^{(X)}$	5.4	6.27 [8]	4.41, 5.37 [8]	4.56	4.52 [8]	3.2, 4.7 [8]
RI_1	2.11	2.12 [9]	1.23-2.45 [9]	2.21	2.24 [11]	2.07-2.41 [11]
RI_2	2.35	2.10 [10]		2.46	2.40 [9, 10]	
RI_3	2.05			2.14		

The energy band gap $E_g^{(X)}$ computed for GaN is perfectly agreed with the experimental findings but some underestimation is observed for BN. The present results of energy band gap $E_g^{(X)}$ are found in better agreement with the experimental results [8] compared to other such theoretical results [8]. The refractive indices computed by Ravindra-Srivastava relation are found in good agreement with the available experimental results [9]. While some overestimation is observed in refractive index computed by Reddy-Ahammed relation and underestimation is found for Moss relation. The variations of the refractive index as a function of gallium concentration over the range 0-1 using three different relations for $B_{1-x}Ga_xN$ are displayed in Fig. 1.

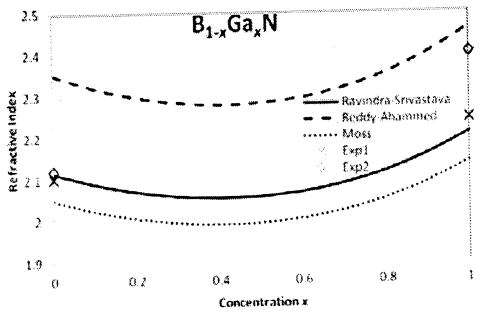

FIGURE 1. Refractive index for $B_{1-x}Ga_xN$.

It is seen from Fig. 1 that refractive index computed by all three relations show same trend in nature, decrease with increasing gallium concentration, minimize for $x = 0.4$, thereafter increase up to $x = 1$ for ternary alloy $B_{1-x}Ga_xN$. It is also observed that the computed refractive index for ternary semiconductor $B_{1-x}Ga_xN$ at $x = 0.4$ is lower in value than the binary parent compounds BN and GaN. The boron compounds display rather peculiar behaviour when compared to other III–V compounds. Their unusual behaviour appears to originate from the small core size and the absence of p electrons in B. Refractive index computed by Reddy-Ahammed relation are higher in values while computed by Moss relation are lower in values for the whole composition range. Present results are found in good agreement at end points. No such experimental results are available for comparison for the entire range of the alloy composition x of ternary semiconductor $B_{1-x}Ga_xN$.

CONCLUSIONS

In the present investigation it is found that the computed energy band gap $E_g^{(X)}$ is satisfactorily agreed with the experimental findings. The refractive index computed by present approach decreases up to gallium concentration $x = 0.4$, thereafter increases with gallium concentration for ternary semiconductor alloy $B_{1-x}Ga_xN$. It is also seen that Moss relation produces lower refractive index, while refractive index computed by Ravindra-Srivastava relation satisfactorily agree with the experimental findings. As per the best of our knowledge, such a theoretical study of the refractive index with gallium concentration for $B_{1-x}Ga_xN$ is the first time reported in this paper. Overall our results using novel model potential are satisfactory and could be used for further comprehensive study of such semiconductor system.

ACKNOWLEDGMENTS

The author P. S. Vyas is thankful to UGC, New Delhi, India for providing financial support under minor research project No. F. :47-651/08(WRO).

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AIP Conference Proceedings

Elastic constants and pressure derivative of elastic constants of Si1−xGex solid solution

A. R. Jivani, J. K. Baria, P. S. Vyas, and A. R. Jani

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Elastic Constants and Pressure Derivative of Elastic Constants of $Si_{1-x}Ge_x$ Solid Solution

A. R. Jivani[1], J K Baria[1], P S Vyas[1] and A. R. Jani[2]

[1]*Physics Department, VP & RPTP Science College, Vallabh Vidyanagar-388 120, Gujarat, India*
[2]*Department of Physics, Sardar Patel University, Vallabh Vidyanagar-388 120, Gujarat, India*
E-mail ID: jivani_a_r@yahoo.com

Abstract. Elastic properties of $Si_{1-x}Ge_x$ solid solution with arbitrary (atomic) concentration (x) are studied using the pseudo-alloy atom model based on the pseudopotential theory and on the higher-order perturbation scheme with the application of our own proposed model potential. We have used local-field correction function proposed by Sarkar et al to study Si-Ge system. The Elastic constants and pressure derivatives of elastic constants of the solid solution is investigated with different concentration x of Ge. It is found in the present study that the calculated numerical values of the aforesaid physical properties of Si-Ge system are function of x. The elastic constants (C_{11}, C_{12} and C_{44}) decrease linearly with increase in concentration x and pressure derivative of elastic constants (C_{11}', C_{12}' and C_{44}') increase with the concentration x of Ge. This study provides better set of theoretical results for such solid solution for further comparison either with theoretical or experimental results.

Keywords: Pseudopotential method, $Si_{1-x}Ge_x$ solid solutions, the pseudo-alloy atom model, elastic constants, pressure derivatives of elastic constants .
PACS: 64.70.kg, 62.20.de, 71.15.Dx

INTRODUCTION

Previously, we have successfully reported the application of Jivani *et al* [1-7] potential to investigate some physics properties of semiconductors like Group IV, Group III-V, Group II-VI and their alloys [1-7]. The results generated are generally in good agreement with experimental values and available other theoretical values. The application of the potential proposed by Jivani et al [1-7] is extended in the present work to investigate elastic constants and pressure derivative of elastic constants of the $Si_{1-x}Ge_x$ solid solutions with arbitrary (atomic) concentration x of Ge. The Si-Ge system is interesting due to application of such system in optoelectronics devices.

In present work, we have used pseudo-alloy atom model [7] (hereafter referred to as PAA) alongwith homogeneous deformation method [4] to investigate elastic constants and pressure derivatives of elastic constants at different concentration of $Si_{1-x}Ge_x$ system with concentration x of Ge. For the incorporation of exchange and correlation effects to the dielectric function, we have adopted Sarkar *et al* approximation [8] to consider exchange and correlation effect.

COMPUTATIONAL METHOD

In the higher-order perturbation theory, the total energy of the crystal per atom [1-7] is given by

$$E = E_i + E_0 + E_1 + E_2 + E_{cov} \quad (1)$$

In equation (1), E_i is electrostatic energy of point ions in the uniform gas of valence electrons, E_0 is the sum of the kinetic, exchange and correlation energies of the valence electron, E_1 is the first-order perturbation energy of the valence electron due to the pseudopotential, E_2 is the second-order perturbation term and E_{cov} is the covalent correction term. The detailed expressions of the energy terms used in equation (1) are given in reference [1].

In the pseudo-alloy atom model, a hypothetical monoatomic periodic lattice is replaced by the disordered alloy [7]. The screened potential form factor $W_s^{PAA}(q)$ of an electron with a single PAA in the case of solid solution is given by

SOLID STATE PHYSICS: Proceedings of the 57th DAE Solid State Physics Symposium 2012
AIP Conf. Proc. 1512, 1062-1063 (2013); doi: 10.1063/1.4791411

$$W_s^{PAA}(q) = -\frac{12\pi Z^{PAA\ 2} e^2}{\Omega q^3 R_c^{PAA} \varepsilon(q)} \left[\frac{\sin(q R_c^{PAA})}{2} - \frac{1}{q R_c^{PAA}} + \frac{\sin(q R_c^{PAA})}{(q R_c^{PAA})^2} \right] \quad (2)$$

In equation (1), ε(q) is the static Hartree dielectric function, $Z^{PAA} = Z^{Si} = Z^{Ge} = 4$ is ion valency, e is the electronic charge, Ω is the atomic volume, q is the wave vector and R_c is the parameter of the potential.

The value of model parameter R_c for a single element is determined by fitting the experimental bulk modulus of the system. The parameter

$$R_c^{PAA}(x) = (1 - x) R_c^{Si} + x R_c^{Ge}. \quad (3)$$

The elastic constants and pressure derivative of SiGe solid solution is calculated using above average screened potential and model parameter as defined in equation (3).

RESULTS AND DISCUSSION

In Figure 1, we have shown the elastic constants (C_{11}, C_{12} and C_{44}) of solid solution SiGe using PAA model investigated using Sarkar *et al* [8] screening function with different concentration x of Ge.

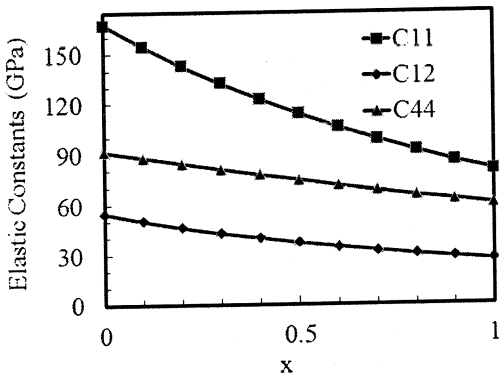

FIGURE 1. The elastic constants of SiGe system as a function of concentration (x) of Ge.

Figure 1 show the variation of the elastic constants with concentration x. For a particular x, the magnitude of C_{11} is the highest, the lowest in the case of C_{12} and intermediate in the case of C_{44}.

The elastic constants decrease with increase in concentration x of Ge. The linear relation between calculated elastic constants and concentration x with the application of Sarkar et al [8] screening function:

$$C_{11} = -86.486x + 161.29 \quad (4)$$
$$C_{12} = -27.64x + 52.331 \quad (5)$$
$$C_{44} = -31.329x + 90.695 \quad (6)$$

As shown in Figure 2, the pressure derivative of elastic constants are function of concentration x. The elastic constants decrease with increase in concentration x of Ge.

As far as our knowledge, no such work had been reported earlier and hence the comparison of our results with the experimental and theoretical results is difficult.

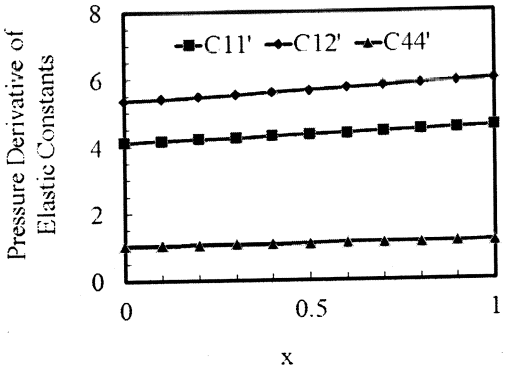

Figure 2. The pressure derivative of elastic constants of SiGe system as a function of concentration (x) of Ge.

CONCLUSION

Thus, elastic properties of Si-Ge solid solutions are studied employing the present formulation of model potential [1-7] with the higher-order perturbation theory and the pseudo-alloys atom model This work represents the elastic behavior which will surely lead to a better understanding of the physical properties of Si-Ge solid solution.

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LASER welding Process for RF Connectors for Space Applications

Sakaram Srinivasulu[1], Shivendra Tripathi[2], R.K. Hegde[3], J K Baria[4]
Space Applications Centre-ISRO Ahmedabad, V.P.R.P.T.P. Science College, Sardar patel University
Vallabh Vidyanagar Gujarat, India

Abstract*—LASER (Light Amplification by Stimulated Emission of Radiation) welding of RF (Radio Frequency) connectors & DC (Direct Corrent) feedthrough finds potential applications in aerospace and defence where environmental conditions require extremely rugged and reliable weld joints. Present paper is focused on the application of Nd: YAG (Niobdenum-Yitrium Aluminum Garnet) LASER at 1064 nm wavelength for welding of RF & DC connectors with A16061 and characterization of weld joint in terms of environmental, mechanical & RF leakage tests for possible use in aerospace hardware. Using optimized laser weld parameters, welding of RF connectors and DC feedthrough with AI 6061 flange have been completed. Leak rate of <1x10^{-7} Atm cc/Sec Helium has been demonstrated successfully using sniff leak test method for all the seven samples which indicates good process repeatability. The laser weld joint has withstood various Environmental tests namely Thermal shock -70° C to + 180° C with dwell time of 10 min for each extreme for total of 500 cycles and Sine & Random vibration tests and passed the post environmental leak tests which is in conformance with MIL-STD-883 requirements. The Mechanical load test for weld joint strength showed no failure even at 23.2 kgf, which indicates the robustness of the joint. The micro sectioning of the joint indicates the depth of penetration of approximately in the range 280-300 microns for the optimized laser energy levels. Further the radiography analysis has been carried out which indicates crack free and uniform weld joint.

Keywords- LASER Welding, RF Connector , DC Feedthrough, He Leak Test, Weld qualification, Thermal Cycle, Vibration, Heat Affected Zone (HAZ)

I. INTRODUCTION

The technological approach involves application of laser beam welding to hermetically seal LASER weldable RF connector and DC Feedthrough, with AI6061 alloy.

Better control on laser weld process parameters such as pulse to pulse overlap, beam energy etc. helps in the realization of a weld joint with leak rate levels <1x10^{-7} Atm cc/Sec He.

Being low Heat Affected Zone (HAZ)[1], it produces a metallurgical fusion weld in a small localized area at the interface. This development eliminates the otherwise mandatory need of Gold plating inside connector holes and use of mechanical fasteners.

Laser weldable RF connector/DC feedthrough housing basically consists of an outer shell made up of A14047 alloy and the contact pins are isolated from the body by means of an insulator. The use of A14047 as an outer shell has two distinct advantages namely, first it makes the Connector body laser weld compatible with A16061 and second, it saves 30 to 50% weight over its conventional counterparts made up of Kovar or Stainless steel.

The objectives of these experiments were

- To develop the LASER weld process for Weldable Feed through & RF connector assembly on Aluminium packages for RF applications.
- LASER weld process qualification for space usage.

Literature survey has been carried out on the use of Nd-YAG laser for welding of Al alloys [2-4].

II. LASER WELD PROCESS DEVELOPMENT & OPTIMIZATION

The Laser Hermetic Sealing System with Nd-YAG [5] laser has been used. The system comprises of Laser power supply, Glove box and a drier unit integrated with necessary electrical and electronic interfacing. The Glove box housing includes stage assembly for sample mounting with spring loaded mechanism, provision for Fiber Optic Beam Delivery (FOBD) at the work piece and provision

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for soot sucker among others. The Principle of Laser welding is shown below in Figure-1.

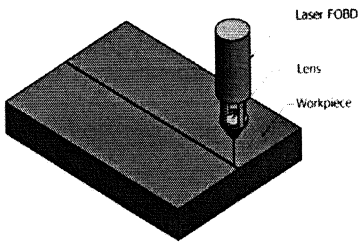

Figure-1 Principle of Laser welding

Here, the Glove box is continuously purged with High purity 99.999% inert Argon gas -also called as carrier gas, in order to lower moisture and oxygen ppm levels suitable for laser weld process.

Weld surface cleaning of Aluminium alloy and RF laser weldable connector and laser weldable Feedthrough are performed using a soft tissue brush, followed by Iso Propyl Alcohol (IPA) solvent cleaning to remove contamination.

Mechanical geometric requirements for joint configuration of weld package & outer shell interface tolerance requirements are presented in Table-1 below.

TABLE I. MECHANICAL REQUIREMENTS

Parameter/Description	Optimal requirements
Package Material	AI6061 alloy
Connector Outer shell	AI4047
Outer shell Thickness	1 to 2.0 mm
Interface gap	Range: 50 to 100 +/- 10 microns uniform throughout weld area/contour.
Interface Co-planarity	Up to +70 microns
Outer Shell Dimension (DC & RF)	8- 10 mm Ø

Laser Weld Process parameter optimization-

Laser weld process parameters [6] have been optimized for Laser welding of weldable RF connector & DC feedthrough with AI6061 alloy package, by carrying out several laser weld iterations. The relation between laser energy (E), peak power (P) and pulse width (W) is -

$$E = P \times W$$

Prior to the laser weld the packages has been subjected to the demoisturisation cycle in a vacuum oven for specified temperature and duration. High purity Argon gas has been used to purge the Glove box. The laser weld process has been carried out in a Glove box. Smooth weld was achieved under optimal values (as per table-2) without any spiking/spattering defects . Laser welded RF connector image and weld geometry are given in figures 2 & 3 respectively.

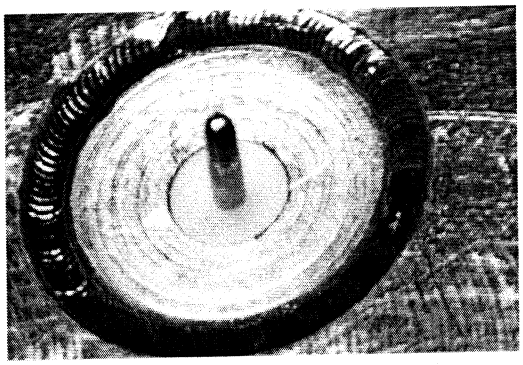

Figure-2 Laser welded RF Connector

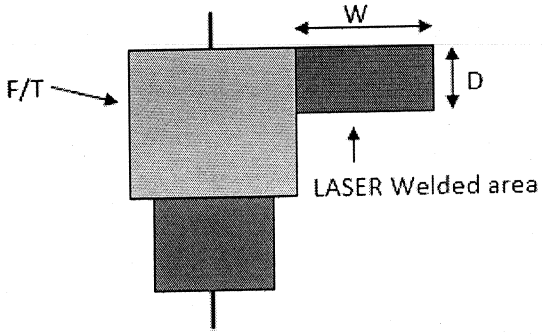

Figure-3 Weld Geometry

Optimized process parameters of the experiment are presented in Table -2 below.

TABLE-2 LASER WELD PROCESS PARAMETERS

Laser parameter	*Range*
Peak power	1.5 – 3.0 KW
Pulse width	3 – 10 ms
Pulse repetition rate	10—20 Hz
Travel speed	1 -4 mm/sec

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Typical laser weld Process sequence flow chart is shown in figure-4

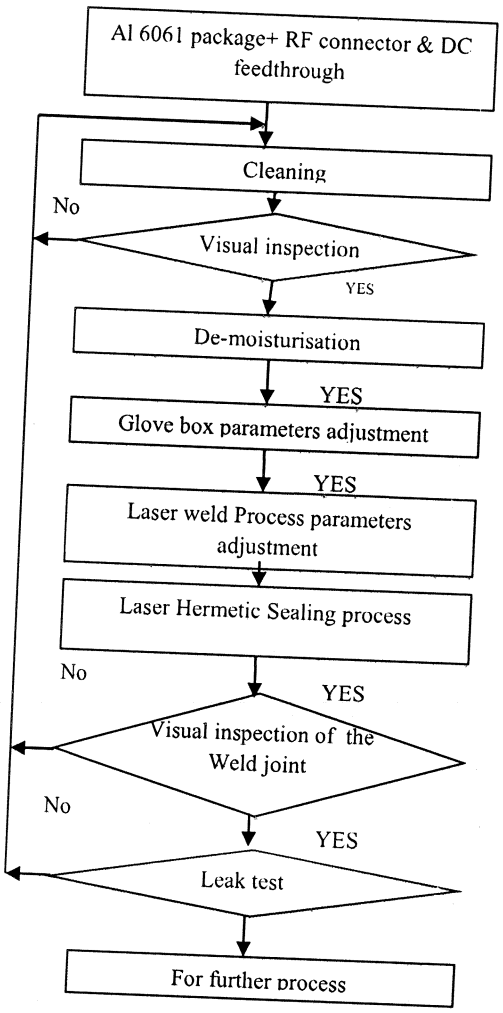


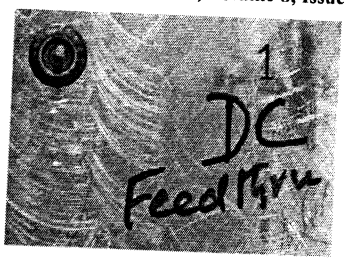
Figure-4 Laser Weld Process Chart

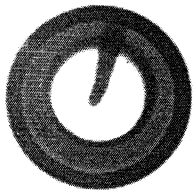
Laser welded RF connector & Feedthrough

Figure-5 gives the visual and X-ray micrograph of the laser welded RF connector and DC feedthrough using optimized laser process parameters, under controlled glove box environmental conditions.

It shows typical weld segments as well as X-ray NDT image of welded RF connectors.

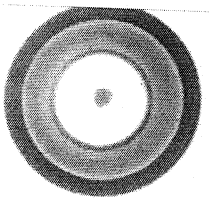
It is clear from these figures that the weld uniformity [7] is consistent which suggests good process repeatability throughout the perimeter under optimal conditions [8].





LASER Welding-DC feedthrough

X Ray Micrograph



LASER Welding-RF Connector

X Ray Micrograph

Figure-5: Visual & X Ray Micrographs

III. PRE WELD INSPECTION

A. Visual inspection:

Pre weld joint interface dimensional requirements are as per Table-1. Proper part mating & positioning is critical for the success of the weld joint. The gap between AI6061 and connector outer shell interface is optimized at 50 to 100 μ ± 10 μ for the development of laser welding process. This is consistent with the pre-weld joint interface requirement reported in the standards [9, 10].

B. Electrical measurement:

Laser welded RF connector

Preliminary electrical checks have been carried out before laser welding of RF connectors. Resistance measurements between Connector centre pin and the outer shell of the body shows 'open' connection.

Laser welded DC feedthrough

Preliminary electrical checks have been carried out before laser welding of DC feedthrough. The DC measurement indicates resistance value as 'open' between the connector-centre pin and the outer shell of the body. No deviation has been found in the post weld measurements.

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Further, the measured capacitance value using LCR meter bridge, was in the range of 9000-10000 pf .

IV. POST WELD INSPECTION & SAMPLE TESTING

Visual inspection:

Post weld joint inspection has been carried out at 40X to confirm the weld quality and absence of defects like pin hole, cracks, blow hole etc.

Electrical measurements:

Laser welded RF connector

Electrical checks have been carried out after laser welding of RF connectors. The resistance probe indicated 'open' connection between the connector centre pin and the outer shell of the body.

Laser welded DC feedthrough

Electrical checks have been carried out after laser welding of DC Feedthrough. The DC measurement indicates resistance value as 'open' between the connector-centre pin and the outer shell of the body & there is no change in the measured capacitance value as compared to pre weld capacitance value.

Mechanical load Tests :

The Mechanical load test on the weld joint strength showed no failure even up to 23.2 Kgf, which indicates the robustness of the joint.

Environmental tests:

Pre Environmental leak test

Sniff leak test has been carried out using Varian Leak detector of laser-welded samples as per the standard procedure. The measured pre-environmental leak rate was $<2x10^{-8}$ Atm cc/sec He against the required specification of $<1x10^{-7}$ Atm cc/sec He.

Post Environmental tests:

1-Thermal Cycling

Laser welded samples have been subjected to thermal cycling for 500 thermal cycles, as per the duration shown in Figure 6

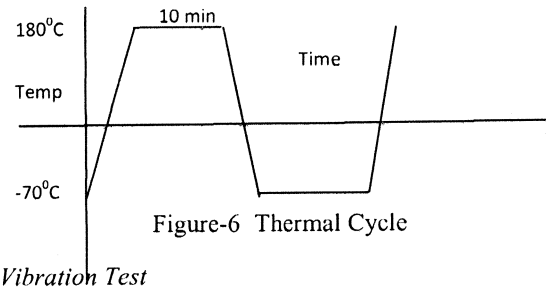

Figure-6 Thermal Cycle

2-Vibration Test

Laser welded samples have been subjected to vibration levels. The dosage levels and sequence followed are given in Table -3.

TABLE-3 VIBRATION LEVELS

Sine Vibration	
In plane	15g
Normal Plane	20g
Random Vibration	
In plane	11.8grms
Normal Plane	17.5grms

Leak test :

Post environmental tests (thermal & vibration), Helium sniff leak rate test measurements were carried out and the results are tabulated in Table-4.

TABLE-4 LEAK RATE MEASUREMENTS

Test Event	Leak Rate Atm cc/sec.He	
	RF Connector	DC Feedthrough
Pre Environmental	$<2x10^{-8}$	$<2x10^{-8}$
Post Thermal Cycling	$<2x10^{-8}$	$<2x10^{-8}$
Post Vibration	$<2x10^{-8}$	$<2x10^{-8}$

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X-ray analysis:

After the environmental tests, X ray analysis has been carried out to detect fine crack/discontinuity. The samples were found free from such defects. Fig 7 shows the x-ray image for DC Feedthrough.

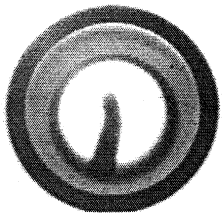
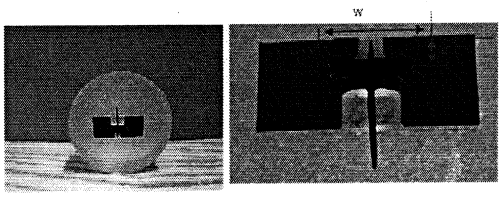


Figure-7 Xray Micrograph- DC Feedthrough

Micro section Analysis:

After the qualification tests, micro sectioning of weld joint was carried out. Measured value of depth of penetration was reported to be in the range of 280-300 μ (D) and that of width (Heat Affected Zone) is approximately 817 μ (W) for the optimized laser energy levels for fiber core diameter of 600 μ.

Research survey indicates that depth of penetration is linked to the key hole weld process[11-13]. Further, the micro-section analysis has been carried out, which indicates crack free and uniform weld joint as shown in Figure 8



Figrure-8 Micro-section analysis

These have been successfully implemented in realization of GEOSAT flight packages for Ku-ALC Driver amplifiers.

V. CONCLUSION

The major outcomes of these experiments are as follows

- Weld package-connector outer shell interface geometrical tolerance has been successfully optimized.
- Laser welding process for RF connector and DC feedthrough with A16061 package, has been successfully developed & optimized using Nd-YAG laser.
- Process repeatability has been demonstrated through qualification tests.
- Laser welded RF connector & DC feedthrough passed environmental leak test & results are meeting MII-STD-883 standards specification < $1x10^{-7}$ Atm cc/secHe for hermeticity requirement for space applications for MMIC based RF subsystems.

Being a metallurgical fusion bonding, LASER weld technology promises potential applications [14] for the packaging & sealing of microelectronic space hardware for geostationary as well as interplanetary outer space missions, having extreme thermal excursion. The developed process had been a precursor for complex/precision part welding such as Multipin Micro D connectors on aluminum packages.

These have been successfully implemented in realization of GEOSAT flight packages for Ku-ALC Driver amplifiers.

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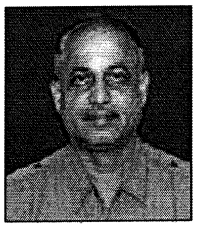
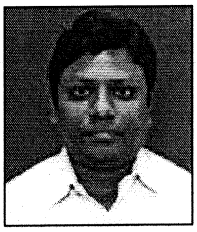
ACKNOWLEDGEMENTS

Authors would like to thank teams at MESA, SNPA EnTSG and SRG in Space Applications Centre, for their constant guidance and support at every stage of this activity. The activity would not have been possible without support from Microelectronics assembly division's support.

AUTHOR's BIOGRAPHY



Sakaram Srinivasulu did his M.Sc., M.Phil. , in Physics and worked on R&D projects in thin film devices at IISc., Bangalore prior to joining SAC/ISRO Ahmedabad in the year 1992. He has developed expertise on LASER hermetic sealing technology, which is qualified and implemented for delivery of FM hardware for all GEOSAT missions, Presently, he is working on the development of advanced Wafer level packaging technology and LTCC assembly & packaging. (srinivasulu@sac.isro.gov.in)



Shivendra Tripathi did his B.Tech. in Electronics & communication from J.S.S. Academy, Noida. He is with Space Applications Centre (ISRO) since 2006. He is presently leading the team responsible for MIC/MMIC Assembly activities at MAPD/MEG for SAC. He has developed new fabrication processes for fine pitch, SMT & Area Array Device assembly processes which have been qualified and implemented for space-borne payloads. He has worked extensively for establishment of advance packaging & assembly facility. (*shivendra@sac.isro.gov.in*)

R. K. Hegde did his BE in Electronics & Communication Engineering from LDCE Ahmedabad, and is presently leading quality assurance activities as Head PMQD(E)/SRG, at Space Applications Centre. He has been a Failure Analyst for 20 years and has been Process QA Engineer for 11 years. (*rkhegde@sac.isro.gov.in*)

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Dr J.K. Baria did his Ph.D. in Physics from Sardar Patel University, Vallabhvidyanagar. He is an Associate Professor at Department of Physics at V.P. R.P.T.P Science College. He has developed expertise in theoretical simulation & modelling of Solids. He has authored several research papers published in national/international journals. (*jkbaria0110@gmail.com*)

Theoretical Investigations of transition metals and their binary alloys using ab-initio Pseudopotential Theory

A project proposal submitted to the
University Grants Commission (UGC)
For

MAJOR RESEARCH PROJECT

By

Dr. M. H. PATEL (P. I.)
&
Dr. J. K. BARIA (Co-I.)

V. P. & R. P. T. P. Science College
Vallabh Vidyanagar 388 120
Gujarat State

FORMAT FOR SUBMISSION OF PROPOSAL FOR

MAJOR RESEARCH PROJECT

PART – A

1.	Broad Subject	:	**Physics**
2.	Area of Specialization	:	**Computational condensed matter physics**
3.	Duration	:	**Three Years**
4.	Principal Investigator		
i.	Name	:	**Dr. M. H. Patel**
ii.	Sex: M/F	:	**Female**
iii.	Date of Birth	:	**24th June, 1967**
iv.	Qualification	:	**M. Sc., M. Phil., Ph.D.**
v.	Designation	:	**Associate Professor in ELECTRONICS**
vi.	Address	:	
	Office	:	**Dr. M. H. Patel, Lecturer in Electronics** **V. P. & R. P. T. P. Science College** **Vallabh Vidyanagar – 388 120** **State: Gujarat**
	Residence	:	**7, Rajesh Society,** **Bhaikaka Marg** **Vallabh Vidyanagar – 388 120** **State: Gujarat**
5.	Co – Investigator(s):		
i.	Name	:	**Dr. J. K. Baria**
ii.	Sex: M/F	:	**Male**
iii.	Date of Birth	:	**1st October, 1968**
iv.	Qualification	:	**M. Sc., M. Phil., Ph. D.**

v. Designation : **Associate Professor in PHYSICS**

vi. Address:

Office : **Associate Professor in PHYSICS**

V. P. & R. P. T. P. Science College

Vallabh Vidyanagar – 388 120

State: Gujarat

Residence : **A-1/3, Ashirwad Society**

B/H Nilkamal Society, Karamsad Road

Vallabh Vidyanagar – 388 120

State: Gujarat

6. In case of a retired teacher, please give the following information:

(i) Date of Superannuation:

ii. Age at the time of Superannuation:

iii. Whether employed or not

7. Name of the Institution where the project will be undertaken:

(a) Department: -

b. University/College: **V. P. & R. P. T. P. Science College,**

Vallabh Vidyanagar – 388 120

Affiliated to Sardar Patel University Vallabh Vidyanagar – 388 120

(Please mention the name of affiliating University in case of college)

8. Whether the University/College/Institution is approved under Section 2 (f) and 12 (B) of the UGC Act?

Yes/No : **Yes**

9. Teaching and Research Experience of Principal Investigator :

a. Teaching experience : **TWENTY ONE YEARS**

b. Research experience : **TWENTY ONE YEARS**

c. Year of award of Doctoral degree : **2002**

(d) Title of thesis for doctoral degree :

Dr. M. H. Patel's Thesis title : "Theoretical Investigations of transition metals and their binary alloys using Pseudopotential Theory"

Dr. J. K. Baria's Thesis title: "Study of Certain Physical Properties of d and f –shell metals Using Pseudopotential Theory"

e. Publication: **See Appendix – A**

Dr. M. H. Patel's

i. Papers Published :

Accepted : **01**

Communicated : **02**

ii. Books Published :

Accepted : **00**

Communicated : NIL

Dr. J. K. Baria's

ii. Papers Published :

Accepted : **19**

Communicated : **07**

iii. Books Published :

Accepted : **03**

Communicated : NIL

(Please enclose the list of papers and books published and/or accepted during last five years)

See Appendix - A

PART – B

Proposed Research Work

10. (i) Project Title :

"Theoretical Investigations of transition metals and their binary alloys using ab-initio Pseudopotential Theory"

(ii) Introduction : **See appendix - B**

- Origin of the research problem
- Interdisciplinary relevance
- Review of Research and Development in the Subject:
  - International status
  - National Status
  - Significance of the study

(iii) Objectives : **See appendix - B**

(iv) Methodology : **See appendix - B**

(v) Year wise Plan of work and targets to be achieve. : **See appendix - B**

(vi) Details of collaboration, if any intended : Yet not decided

Summary of research Proposal

"Theoretical Investigations of transition metals and their binary alloys using ab-initio Pseudopotential Theory"

The advent of simple metals, non-simple metals, noble metals, transition metals, alkaline earth elements, lanthanide elements, and semiconductors and their compounds and alloys have been one of the most exciting events in the field of materials science and industry. Particularly, it is found that such study during the last decades is contributing immensely in the field of materials generates manifold interest for experimentalist as well as theoreticians. These elements show remarkable and widespread applications. Besides the experimental work on these elements, their compounds and alloys there have been little theoretical efforts because of the computational difficulties and complexities that arise in dealing with the order and disorder in the systems. By applying an ab-initio Pseudopotential theory one can overcome the complexities of computations and investigate various static, dynamic, electronic and thermodynamic properties. It has been notice from the literature that the concept of Pseudopotential is well established in the theory of condensed matter, which helps us in understanding various properties including physical as well as chemical properties of crystalline and amorphous materials. It is also established that a proper and well-stabilized Pseudopotential yields much better and easier way for predicting different properties of crystalline solids with higher accuracy using various software like Wien2K, VASP, Phonon, Crystal09 and Quantum Espresso.

Hence looking to the ease of Pseudopotential formalism we have felt it worthwhile to undertake a research project leading to a comprehensive study of ordered and disordered materials using ab-initio Pseudopotential Theory with the help of proposed computing facility, man power and financial assistance.

The work will pay attention to mainly the following objectives:

- To identify the ab-initio Pseudopotential, which can be used in the present investigation.
- To explore the ab-initio Pseudopotential in the study of various physical properties in the ordered and disordered form of
  - Transition metals
  - Compounds and alloys of these metals and elements
- To carry out the theoretical investigations of various physical properties using ab-initio Pseudopotential with second order perturbation scheme.
- To predict the usefulness of various simulation techniques in the study of binary and ternary compounds & alloys.
- To investigate the impact of various exchange and correlation functions in the aforesaid study.

These theoretical investigations may include the computation of Equation of State (EOS) namely, the relationship "among" Pressure-Volume-Temperature i.e. (P, V, T) investigation, phonon dispersion curves in q-space, phonon density of states (PDOS), various physical properties which can be obtained from the PDOS such as Debye-Waller Factor, Mean-square displacement, Dynamical elastic constants, deviation from Cauchy's relation, Poisson's ratio, Young modulus and propagation velocities of elastic waves. We may also calculated structure dependent properties of liquid metals at various temperatures such as Dynamical elastic constants, Velocity autocorrelation function, Diffusion coefficient, Phonon dispersion curves, Characteristic frequency, Power spectrum, Viscosity and Surface tension of these metals their compound and alloys, using various software like Wien2K, VASP, Phonon, Crystal09 and Quantum Espresso.

We have made some collaboration with the various PG Departments of Gujarat, Which includes Sardar Patel University, Gujarat University, Saurastra University and Veer Narmad South Gujarat University, we have also made a collaboration with IIT's of Delhi, Mumbai and Kanpur, BARC-Mumbai, Institute of Physics Bhubaneswar.

We would like to stress here that the experimental work on the thin film and in the bulk form of some of the above systems is extensively going on in our post graduate department as well as in other post graduate departments of our University. This also includes the development of electrical resistivity in semiconductor at high pressure. Therefore we believe that some of our theoretical investigations would be immensely helpful in giving physical interpretation to theoretical and experimental results from both the groups of the department and University.

Both the investigators are well trained in the academic administrations and Research hence the investigators do not find any serious hurdles in completing successfully the proposed project.

Year wise Plan of work and targets to be achieve

Year	Work
1st	We plan to investigate various physical properties of Transition metals in ordered states. For this necessary literature survey would be made. Appointment of the project fellow will be done. Necessary codes of the computations will be developed along with the modifications in existing coeds. Computations for the system of transition metals in order states will be carried out. Sanction equipments and necessary books will be purchased.
2nd	We plan to investigate various physical properties of Transition metals in disordered states. The results of transition metals will be communicated in new publications and additional physical properties of transition metals in disorder states will be studied theoretically – and analytically as well as through computations. Obtained results will also be presented in possible seminar, symposia, conferences etc..
3rd	We plan to investigate various physical properties of Transition metals, their binary alloys. In the last year we would focus to complete the project successfully while applying the above developed techniques to the binary alloys of transition metals. Results will be published along with their presentation in possible seminar, symposia, conference etc..

(Dr. M. H. Patel)
Principal Investigator &
Associate Professor in Physics
V. P. & R. P. T. P. Science College
Vallabh Vidyanagar 388 120

(Dr. J. K. Baria)
Co. Investigator
Associate Professor in Physics
V. P. & R. P. T. P. Science College
Vallabh Vidyanagar 388 120

(Dr. Bhavesh D. Patel)
Principal,
V. P. & R. P. T. P. Science College,
Vallabh Vidyanagar 388 120

PRINCIPAL
V.P.&R.P.T.P.SCI. COLLEGE
VALLABH VIDYANAGAR-388120

V. V. Nagar 388 120

Financial Assistance required

Budget in Rupees for recurring				
Item	1st Year	2nd Year	3rd Year	Total
Salaries/Wages One Project associate @ Rs14000/- p. m. (fixed)	1,68,000/-	1,68,000/-	1,92,000/-	5,28,000/-
Hiring Servises	10,000/-	10,000/-	10,000/-	30,000/-
Field Work and Travel	10,000/-	10,000/-	10,000/-	30,000/-
Chemicals and glassware	-	-	-	-
Contingency (including special needs)	20,000/-	20,000/-	20,000/-	60,000/-
Honorarium to retired teacher @Rs. 10,000/-	-	-	-	-
Books and Journals	15,000/-	15,000/-	15,000/-	45,000/-
Total of recurring items				6,93,000
Budget in Rupees for nonrecurring				
Equipments: One Desk-top Computers + One Lap-top Computer, One Laser Printer (Multifunction) UPS + other peripherals with provision of time to time up gradation and maintenance.				3,00,000/-
Software: For advanced Calculation of some physical properties we need the software like, Wien2K, VASP, Phonon, Phon, Crystal09, quantum espresso etc.,				3,50,000/-
Total of non recurring items				6,50,000/-
Total of recurring + non recurring budget				13,43,000/-

10% of the Total Budget proposal i.e. Rs. 1,34,300.00 should be the overhead charges as per the resolution of our University syndicate.

Hence TOTAL BUDGET: 13,43,000.00-+ 1,34,300.00= Rs. 14,77,300.00

d. Title of the project for which assistance was approved

e. In case the project was completed, whether the work on the project has been published

f. If the candidate was working for the doctoral degree, whether the thesis was submitted and accepted by the University for the award of degree.

(A summary of the report/thesis in about 1,000 words may please be attached with the application)

g. If the project has not been completed, please state the reasons
(a) Details of the project/scheme completed or ongoing with the P.I

Name of the agency	Year		Total	Equipment/Infrastructural facilities obtained
	Started	Completed		

(b) Institutional and Departmental facilities available for the proposed work:

Equipment:

Other Infrastructural facilities :

16. Any other information which the investigator may like to give in support of this proposal which may be helpful in evaluating.

Appendix - A

Publication of Dr. M. H. Patel

P.N. Gajjar, Minal H. Patel, and A.R. Jani , Computational **material science 42, 316 (2008).** Asphericity in the Fermi surface and Fermi energy of $Li_{1-x}B_x$(B= Na, K, Rb and Cs) substitutional alloys ,

Publication of Dr. J. K. Baria

List of Publication in International Journals

1. J. K. Baria, and A. R. Jani, **J. of Non-Crystalline Solids 356, 1696-1702(2010),** Molecular dynamics of liquid alkali metals near melting temperature.
2. J. K. Baria, and A. R. Jani, **Indian Journal of Physics 84, 1509-1516 (2010),** The effect of temperature on elastic constants and bulk modulus.
3. J. K. Baria, and A. R. Jani, **Pramana 75, 737-748 (2010),** Molecular Dynamics of liquid alkaline-earth metals near melting point temperature.
4. J. K. Baria, and A. R. Jani, **Digest J. of Nanomaterials and Biostructures, 5/2, 317-322 (2010),** Enthalpy, Entropy and Helmholtz free energy of transition and rare earth liquid metals.
5. J. K. Baria, and A. R. Jani, **Brazilian j of Physics 40, 204-209 (2010),** Structural Studies of Liquid Alkaline-earth Metals -A Molecular Dynamics Approach.
6. J. K. Baria, and A. R. Jani, **Digest J. of Nanomaterials and Biostructures, 5, 23-27 (2010),** New criteria for the selection of exchange and correlation function.
7. J. K. Baria, and A. R. Jani, **Physica B: Condensed Matter, 405, 2065-2071 (2010),** Lattice Dynamics of La, Yb, Ce and Th.
8. J. K. Baria, and A. R. Jani, **Physica B: Condensed Matter, 404, 2401-2411 (2009),** Lattice mechanical properties of alkaline earth metals in bcc and fcc Phase.

9. J. K. Baria, and A. R. Jani, **Turk J Phys 33, 81 (2009),** Asphericity in the Fermi Surface of d and f-shell metals.
10. J. K. Baria, and A. R. Jani, **Moroccan J Of Phys. : Condensed Matter, 11, 09 (2009),** Contribution of a point defect to the electrical resistivity of simple and non-simple metals.
11. J. K. Baria, and A. R. Jani, **Digest J. of Nanomaterials and Biostructures, 4, 415 (2009),** Magnetic and Electronic properties of simple, transition and rare earth liquid metals.

List of Publication in National Journals

1. J. K. Baria, A. R. Jivani and A. R. Jani, **Structural studies of liquid sodium at various temperatures using molecular dynamics, Solid State Physics Vol. 54, 505 (2009).**
2. A. R. Jivani, J. K. Baria and A. R. Jani, **Dynamical bulk modulus of Si and Ge using higher-order perturbation theory, Solid State Physics Vol. 54, J41 (2009).**

To certify that:

a. The University/College/Institutite is approved under Section 2(f) and 12(b) of the UGC Act and is fit to receive grants from the UGC.

b. General physical facilities, such as furniture/space etc., are available in the Department/College.

c. I/we shall abide by the rules governing the scheme in case assistance is provided to me/us from the UGC for the above project.

d. I/we shall complete the project within the stipulated period. If I/we fail to do so and if the UGC is not satisfied with the progress of the research project, the Commission may terminate the project immediately and ask for the refund of the amount received by me/us.

e. The above Research Project is not funded by any other agency. NO

(Dr. M. H. Patel)
Principal Investigator &
Lecturer in Electronics

(Dr. J. K. Baria)
Co Investigator &
Lecturer in Physics

(Dr. Bhavesh Patel)
Principal
V. P. & R. P. T. P. Science College
Vallabh Vidyanagar 388 120

V. P. & R. P. T. P. Science College V. V. Nagar 388120

APPENDIX - B

SYNOPSIS OF THE PROJECT

Theoretical Investigations of transition metals and their binary alloys using ab-initio Pseudopotential Theory

The advent of simple metals, non-simple metals, noble metals, transition metals, alkaline earth elements, lanthanide elements, semiconductors and their compounds and alloys have been one of the most exciting events in the field of materials science and industry. Particularly, it is found that such study during the last decades is contributing immensely in the field of materials generates manifold interest for experimentalist as well as theoreticians. These elements show remarkable and widespread applications. Besides the experimental work on these elements, their compounds and alloys there have been little theoretical efforts because of the computational difficulties and complexities that arise in dealing with the order and disorder in the systems. By applying a ab-initio pseudopotential theory one can overcome the complexities of computations and investigate various static, dynamic, electronic and thermodynamic properties. It has been notice from the literature that the concept of pseudopotential is well established in the theory of condensed matter, which helps us in understanding various properties including physical as well as chemical properties of crystalline and amorphous materials. It is also established that a proper and well-stabilized pseudopotential yields much better and easier way for predicting different properties of crystalline solids with higher accuracy using various softwares like Wien2K, VASP, Phonon, Crystal09 and Quantum Espresso.

Hence looking to the ease of pseudopotential formalism we have felt it worthwhile to undertake a research project leading to a comprehensive study of ordered and disordered materials using ab-initio pseudopotential Theory with the help of proposed computing facility, man power and financial assistance.

The work will pay attention to mainly the following objectives:

- To identify the ab-initio pseudopotential, which can be used in the present investigation.
- To explore the ab-initio pseudopotential in the study of various physical properties in the ordered and disordered form of
  - Transition metals
  - Compounds and alloys of these metals and elements
- To carry out the theoretical investigations of various physical properties using ab-initio pseudopotential with second order perturbation scheme.
- To predict the usefulness of various simulation techniques in the study of binary and ternary compounds & alloys.
- To investigate the impact of various exchange and correlation functions in the aforesaid study.

These theoretical investigations may include the computation of Equation of State (EOS) namely, the relationship "among" Pressure-Volume-Temperature i.e. (P, V, T) investigation, phonon dispersion curves in q-space, phonon density of states (PDOS), various physical properties which can be obtained from the PDOS such as Debye-Waller Factor, Mean-square displacement, Dynamical elastic constants, deviation from Cauchy's relation, Poisson's ratio, Young modulus and propagation velocities of elastic waves. We may also calculated structure dependent properties of liquid metals at various temperatures such as Dynamical elastic constants, Velocity autocorrelation function, Diffusion coefficient, Phonon dispersion curves, Characteristic frequency, Power spectrum, Viscosity and Surface tension of these metals their compound and alloys, using various softwares like Wien2K, VASP, Phonon, Crystal09 and Quantum Espresso.

International status and Interdisciplinary relevance:

Though more and more number of researcher within the country as well as abroad are concentrating on the investigations pertaining to such systems, the theoretical study based on pseudopotential formulation is very rare. Looking to the industrially and technologically important widespread applications of these metals and their compounds and alloys, the investigators are of the firm opinion that the present research proposal will give some useful results to the community of physics, materials science, engineering and industry. The investigators also emphasize that the work will be beneficial to other experimentalist as well as theoreticians working in this area.

National Status:

Systematic studies on metallic complexes have been the subject of great interest in various Indian Universities and other Institutions also. We have found several publications in this area from IIT's of Delhi, Mumbai and Kanpur, IISc- Bangalore and Kolkatta, BARC-Mumbai, University of Rajasthan - Jaipur, Institute of Physics Bhubaneswar, University of Pune-Pune, Jadavpur University-Kolkatta. Studies on alloys and glasses have been made, in general, on the basis of Ashcroft model or Heine-Abarenkov model. Very few workers have used their own model potential in such investigations. But the comprehensive study on the elements, compounds and alloys is not seen. So application of our model potential in the proposed comprehensive study will definitely add new contribution in the understanding of various properties of elements, compounds and alloys.

Significance of the study:

We would like to stress here that the experimental work on the thin film and in the bulk form of some of the above systems is extensively going on in our post graduate department as well as in other post graduate departments of our University. This also includes the development of electrical resistivity in semiconductor at high pressure. Therefore we believe that some of our theoretical