Final Project Report of UGC Major Research Project for the period **1st October, 2012** to **1st August, 2018**

# "Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"

**F. No. 41-835/2012 (SR)**
Dated: **18th July 2012**

***Submitted To***

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

***By***

***Dr. Jagendra. K. Baria***
**Associate Professor in Physics,**
**Department of Physics**
**V P & R P T P Science College,**
**Vallabh Vidyanagar – 388 120**
**Gujarat**

**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. Jagendra. 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. 41-835/2012 (SR)** dated **18th July 2012**
4. Title of the Research Project : **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"**
5. Effective date of starting the project **1st October, 2012**
6. a. Period of Expenditure: From **1st October, 2012** to **1st August, 2018**
b. Details of Expenditure

| S.No. | | Item | Amount Approved (Rs.) | 1st Instalment | Expenditure Incurred (Rs.) | Balance Amount |
|---|---|---|---|---|---|---|
| i. | Non-recurring | Books & Journals | 50,000/- | 3,00,000/- | 48,007/- | -1,993/- |
| ii. | | Equipment | 2,50,000/- | | 2,48,168/- | -1,832/- |
| iii. | Recurring | Contingency | 75,000/- | 3,86,800/- | 37,461/- | -37,539/- |
| iv. | | Field Work/Travel (Give details in the proforma at Annexure-IV). | 50,000/- | | 48,893/- | -1,107/- |
| v. | | Hiring Services | - | | - | - |
| vi. | | Chemicals & Glassware | - | | - | - |
| vii. | | Overhead | 60,300/- | | 54,159/- | -6,141/- |
| viii. | | Any other items (Please specify) honorarium to Project Fellow | 5,28,000/- | | | -2,01,500/- (Project fellow not appointed) |
| | | Total | 10,13,300/- | 6,86,800/- | 4,36,688/- | -2,50,112/- |

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:**<br>i) **NET/GATE qualified**-Rs. 16,000/- p.m. for initial 2 years and Rs. 18,000/- p.m. for the third year.<br>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. 6,86,000/-** (**Rupees six lakhs eighty six thousands only**) received from the University Grants Commission under the scheme of support for Major Research Project entitled **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"** vide UGC letter No. F. **F. 41-835/2012 (SR)** dated **18th July 2012,** 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. J. K. Baria,**
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

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

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

**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:**

| Name of the Place visited | Duration of the Visit | | Mode of Journey | Expenditure Incurred (Rs.) |
|---|---|---|---|---|
| | From | To | | |
| IIT Kanpur | 18th February, 2012 | 26th February, 2012 | By Air | 35,055/- |
| UGC New Delhi | 11th January, 2012 | 13th January, 2012 | By Train | 6,907/- |
| UGC New Delhi | 28th July, 2015 | 30th July, 2015 | By Train | 6,931/- |
| Total traveling expenditure | | | | 48,893/- |

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

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

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

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

Annexure – V

ज्ञान-विज्ञान विमुक्तये

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

# Utilization Certificate

Certified that the grant of Rs. **6,86,800.00** (Rupees **Six lakhs eighty six thousand and eight hundred only**) received from the University Grants Commission under the scheme of support for Major Research Project entitled **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"** vide UGC letter **No. F. 41-835/2012 (SR)** dated **18th July 2012** 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. **4,36,688/-** ( rupees four lakhs thirty six thousands six hundred eighty eight) and remaining balance of Rs. **-2,50,112/-** (Rupees two lakhs fifty thousand one hundred twelve).

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

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

Harivadan Joshi & Co. * V. V. NAGAR * Chartered Accountants

Signature of the
Chartered Accountant
With Registration number and seal

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

**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 | **50,000/-** | **3,00,000/-** | **48,007/-** | **-1,993/-** |
| ii. | | Equipment | **2,50,000/-** | | **2,48,168/-** | **-1,832/-** |
| iii. | **Recurring** | Contingency | **75,000/-** | **3,86,800/-** | **37,461/-** | **-37,539/-** |
| iv. | | Field Work/Travel (Give details in the proforma at Annexure- IV). | **50,000/-** | | **48,893/-** | **-1,107/-** |
| v. | | Hiring Services | - | | - | - |
| vi. | | Chemicals & Glassware | - | | - | - |
| vii. | | Overhead | **60,300/-** | | **54,159/-** | **-6,141/-** |
| viii. | | Any other items (Please specify) honorarium to Project Fellow | **5,28,000/-** | | | **-2,01,500/-** (Project fellow not appointed) |
| | | Total | **10,13,300/-** | **6,86,800/-** | **4,36,688/-** | **-2,50,112/-** |

It is certified that the grant of Rs **6,86,800.00** (Rupees **Six lakhs eighty six thousand and eight hundred only**) received from the University Grants Commission under the Scheme of support for Major Research Project entitled **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"** vide UGC Letter **No. F. 41-835/2012 (SR)** dated **18th July 2012** 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. **4,36,688/-** ( rupees four lakhs thirty six thousands six hundred eighty eight) and remaining balance of Rs. **-2,50,112/-** (Rupees two lakhs fifty thousand one hundred twelve).

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

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

Harivadan Joshi & Co. V. V. NAGAR Chartered Accountants

Signature of the
Chartered Accountant
With Registration number and seal

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. 41-835/2012 (SR)** dated: **18th July 2012**

Title of the Project: **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"**

| | | | | | | |
|---|---|---|---|---|---|---|
| 1. | Name of the principal investigator | **Dr. Jagendra 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. J. K. Baria**
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

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

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

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

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

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

**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)**

1. Project report.: **Final Report**
2. UGC Reference No.F. **F. 41-835/2012 (SR)** dated **18th July 2012**
3. Period of report: from **1st October, 2012 to 1st August, 2018**
4. Title of research project **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"**
5. (a) Name of the Principal Investigator **Dr. Jagendra. 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 : **1st October, 2012**
7. Grant approved and expenditure incurred during the period of the report:

a. Total amount approved Rs. **6,86,800/-**
b. Total expenditure Rs. **4,36,688/-**
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: **No Difficulties**
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 theproject. 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. J. K. Baria**
(Principal Investigator)
Associate Professor in Physics,
V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

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

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

# Library Accession Certificate

This is to certify that the following books are purchased by Dr. J. K. Baria during his UGC MAJOR RESEARCH PROJECT entitled **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"** [Grant No. **F. 41-835/2012 (SR)** dated **18th July 2012**] and these books are submitted in the college library.

| Sr No. | Title of the book | Author(s) | Publisher | Library accession number |
|---|---|---|---|---|
| 1 | Principles of Condensed Matter Physics | M.P. Chaikin | Cambridge | 49590 |
| 2 | Statistical Mechanics | McQuarrie | Viva | 49591 |
| 3 | Density Functional Theory: A practical introduction | D. S. Sholl | Wiely | 49592 |
| 4 | Ab initio Molecular Dynamics | D. Marx | Cambridge | 49593 |
| 5 | Condensed Matter Physics 2/E | M. P. Marder | Wiely | 49594 |
| 6 | Introduction to Modern Statistical Mechanics | Chandler | Oxford | 49684 |
| 7 | Modern Physics 2/E | Kenneth Krane | Wiely | 50018 |
| 8 | Fundamentals of Time-Dependent Density Functional Theory | Marques, Maitra | Springer | 50019 |
| 9 | Quantum theory of the Solid State: An Introduction | Lev Kantorovich | Kluwer Academic | 50020 |
| 10 | Simulation for Solid State Physics An interactive resources for students | Silsbee Drager | Cambridge | 50021 |
| 11 | The art of Molecular Dynamics Simulation 2/E | Rapaport | Cambridge | 50022 |
| 12 | Molecular modeling principles & applications 2/E | Andrew R Leach | Pearson | 50115 |
| 13 | Equilibrium thermodynamics 3/E | C J Adkins | Cambridge | 50546 |
| 14 | Problems in quantum mechanics with solutions | G. L. Squires | Cambridge | 50547 |

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

**Dr. J. K. Baria**
(Principal 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

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

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

# Assets Certificate

I have submitted the completion report on UGC MAJOR RESEARCH PROJECT entitled **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"** [Grant No. **F. 41-835/2012 (SR)** dated **18th July 2012**] and necessary document to UGC on, February, 2018. I have purchased following items during the project

1. Apple Laptop [MC975HN/A 15" retina i7 2.3 GH/8GBRAM/256GB HDD]
2. Desktop Asus M51c-IN002S 24" LED Display 2TB HDD/8GB RAM/i5 4th Gen
3. Laser printer [HP-1020 plus LaserJet]

I am submitting these items to the college.

**Dr. J. K. Baria**
(Principal 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

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 : **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"**
2. NAME AND ADDRESS OF THE PRINCIPAL INVESTIGATOR **Dr. Jagendra. 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. 41-835/2012 (SR)** dated **18th July 2012**
5. DATE OF IMPLEMENTATION : **1st October, 2012**
6. TENURE OF THE PROJECT : **three years**
7. TOTAL GRANT ALLOCATED : **10,13,300/-**
8. TOTAL GRANT RECEIVED : **6,86,800/-**
9. FINAL EXPENDITURE : **4,36,688/-**
10. TITLE OF THE PROJECT **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"**
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 fully achieved abd 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: **Yes**
17. NO. OF PUBLICATIONS OUT OF THE PROJECT : **04** - See Appendix-C
( PLEASE ATTACH)

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

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

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V P & R P T P Science College,
Vallabh Vidyanagar – 388 120

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

## Objectives of the Project:

**The work will pay attention to mainly the following objectives:**

- 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.

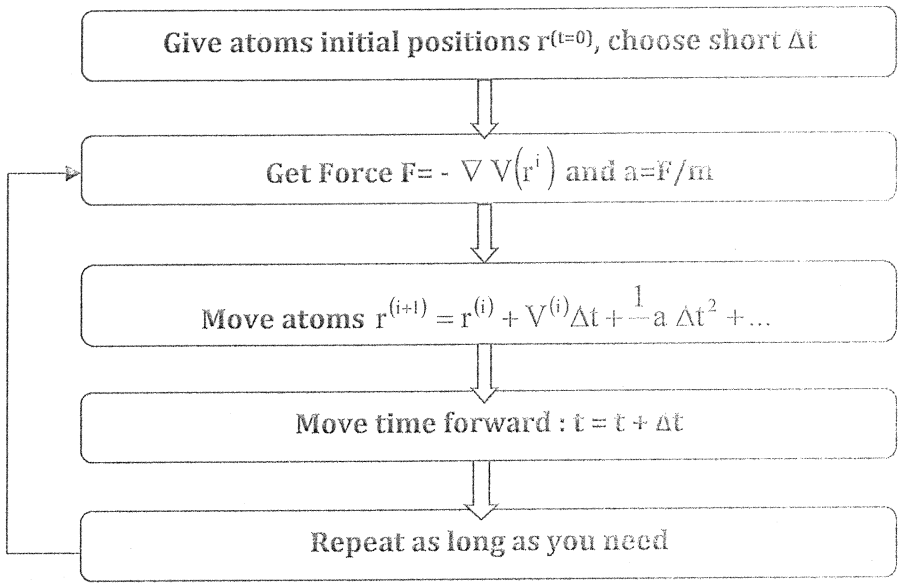
We may also calculated structure dependent properties of liquid metals at various temperatures such as Dynamical elastic constants, Velocity autocorrelation function, Diffusion coefficient, Phonon dispersion curves, Characteristic frequency, Power spectrum, Viscosity and Surface tension of these metals their compound and alloys.

## Methodology:

Molecular Dynamics (MD) is a numerical simulation method calculating the time dependent behaviour of the system. In this technique, the force between atoms are calculated explicitely and the motion of an atom is computed using a suitable numerical integration method, essentially solving Newtonian's equatio of motion. The algorith consists of three essential parts: initialization, equilibrium and production. Initialization requires specifying initial coordinates of the atoms and their velocities. A syastem of n particles initially positioned within a cell of fixed volume, generally cubic in shape. A set of velocities are generated from random numbers, usually selected in such a way as to

make the net momentum zero and its magnitude is scaled to the desired temperature. Following Newton's prescriptions, from the initial positions, velocities and force, it is possible to calculate the positions and velocities of the atoms at small time interval $\Delta t$ (a time step) later. The force are recalculated from these new positions and another step in time is made. The cycle has to be repeated many times in the cource of a full simulation.

**Molecular Dynamics Algoritham**




System comes to equilibrium after a few thousands of the time steps, in which all memory of the initial configuration has been lost and settles down to the desired equilibrium. Then a production period begins in which the trajectory of the atom is stored for later analysis. Many thousands of time steps may be needed to produce a statistically accurate description of a phenomenon of interest. Hence, the thermodynamical properties can be calculated by averaging certain quantities over the equilibrium phase-space trajectory (ensembel average).

MD is a very powerful technique, but has some limitations. MD simulations are restricted by the speed and storage (memory) constraints of the available computers. Hence, simulations are usually performed on systems containing few thousands of atome, and for simulation times ranging from few picoseconds to hundreds of the nanoseconds. Because of the size limitations, a cut-off is applied at certain interatomic separations ($R_c$) and interaction between atoms separated by more than $R_c$ are ignored in the calculations of the atomic forces. However, the imposition of the cut-off gives rise to a break in the continuity of the function at the cut-off distance $R_c$. This introduce the

error in the numerical integration and energy conservation. The cure is to use the shifted potential energy $U(r) = U(r) - U(R_c)$ to control the energy conservation. A limited systen size can also introduce surface effect problem. A solution to this problem is to use periodic boundry conditions (PBC) with minimum image conventions. All the atoms are put inside a box called the unit cell. As an atom goes outside the cell boundry, its image is brought back in from the opposite side of the cell to replace it, and hence the total number of atoms is conserved. Infinite systems may be simulated in this way. Because of the speed limitations, simulations are confined to the studies if the properties having short relaxation time. The relaxation time of the quantities we are interested must be much smaller than the simulation time to get the physical properties accurately.

**List of Publication:**

| Sr No | Title of the paper | Name of Author | Year | Name of the Journal |
|---|---|---|---|---|
| 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 | 2013 | *American Institute of Physics* CP 1536 (2013) 327 |
| 2 | Elastic Constants and Pressure Derivatives of Elastic Constants of $Si_{1-x}Ge_x$ Solid Solutions | A. R. Jivani, **J. K. Baria**, P. S. Vyas and A. R. Jani | 2013 | *American Institute of Physics* CP 1512 (2013) 1062 |
| 3 | Structural Studies of Liquid Rubidium at Various Temperatures Using Molecular Dynamics Simulation Technique | **J. K. Baria**, P. S. Vyas, A. R. Jivani and A. R. Jani | 2012 | *American Institute of Physics* CP 1447 (2012) 535 |
| 4 | LASER welding process for RF connectors for space applications | S Srinivasulu, Shivendra Tripathi, R. K. Hegde, **J. K. Baria** | 2018 | *Int. Journal of emerging Tech. and Advance Engineering (2018) 371* |

**Papers presented in conferences:**

| Sr No | Title of the paper | Name of Author | Year | Name of the Conference | Date |
|---|---|---|---|---|---|
| 1 | Certain Optical Properties of Gallium Based Semiconductors | P. S. Vyas, J. K. Baria and A. R. Jivani | 2014 | 7th National Level Science symposium 2014 on Recent Trends in Science and Technology, Christ College, Rajkot | 23rd February, 2014 |
| 2 | Some Elastic Properties of $Al_xB_{1-x}N$ Semiconductor Alloys | A. R. Jivani, J. K. Baria, P. S. Vyas and A. R. Jani | 2014 | 7th National Level Science symposium 2014 on Recent Trends in Science and Technology, Christ College, Rajkot | 23rd February, 2014 |
| 3 | Certain physical properties of gallium based semiconductors | P. S. Vyas, J. K. Baria and A. R. Jivani | 2013 | National Conference on Condensed Matter Physics and Applications (CMPA 2013), Department of Physics, Manipal Institute of Technology, Manipal University, Manipal | 27th – 28th December, 2013 |
| 4 | 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 | 2013 | International Conference on Recent Trends in Applied Physics & Material Science (RAM2013), Govt. College of Engineering & Technology, Bikaner | 1st – 2nd February 2013 |

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 **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"** vide UGC letter **No. F. 41-835/2012 (SR)** dated **18th July 2012.** by (Dr./Prof./Mr./Mrs.)**Dr. J. K. Baria 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,<br>Department of Physics,<br>M. K. Bhavnagar University,<br>Bhavnagar – 364001<br>Gujarat | 13/8/2018 |
| 2 | Prof. Pankajsinh Thakor | Professor of Physics,<br>Department of Physics,<br>Veer Narmad South Gujarat University,<br>Gujarat | 13/8/2018 |

The proposal is as per the guidelines.

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

(REGISTRAR/ PRINCIPAL)
(Seal)

PRINCIPAL
V.P. & R.P.T.P. SCI. COLLEGE
VALLABH VIDYANAGAR-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 **"Study of some physical properties of transition metals and their alloys using molecular dynamics simulation technique"** vide UGC letter **No. F. 41-835/2012 (SR)** dated **18th July 2012.** by (Dr./Prof./Mr./Mrs.)**Dr. J. K. Baria** 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:**

Major Research Project referenced above has been successfully completed on the line of the proposal by Dr. Jagendra K. Baria, Associate professor in Physics, V.P. & R.P.T.P Sci. Coll., Vallabh Vidyanagar. During the tenure of this project the PI has published 04 research papers in the journals of international repute and presented 04 papers in state level conference; list is attached here with. Papers are based on the theme of the proposal, and we strongly believe that the outcome of the project will definitely add to the domain of condesed matter physics research. We recommend it for further process of complition

**Name & Signatures of Experts with Date:-**

| | Name of Expert | University/College name | Signature with Date |
|---|---|---|---|
| 1 | Prof. N. K. Bhatt | Professor of Physics,<br>Department of Physics,<br>M. K. Bhavnagar University,<br>Bhavnagar – 364001<br>Gujarat | 13/8/2018 |
| 2 | Prof. Pankajsinh Thakor | Professor of Physics,<br>Department of Physics,<br>Veer Narmad South Gujarat University,<br>Gujarat | 13/8/2018 |

It is certified that the final report has been uploaded on UGC-MRP portal on 13th August, 2018.

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.

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

**(Registrar/Principal)**
**Seal**
PRINCIPAL
V.P. & R.P.T.P. SCI. COLLEGE
VALLABH VIDYANAGAR-388120

# Appendix-C

**List of Publication:**

| Sr No | Title of the paper | Name of Author | Year | Name of the Journal |
|---|---|---|---|---|
| 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 | 2013 | ***American Institute of Physics* CP 1536** (2013) 327 |
| 2 | Elastic Constants and Pressure Derivatives of Elastic Constants of $Si_{1-x}Ge_x$ Solid Solutions | A. R. Jivani, **J. K. Baria**, P. S. Vyas and A. R. Jani | 2013 | ***American Institute of Physics* CP 1512** (2013) 1062 |
| 3 | Structural Studies of Liquid Rubidium at Various Temperatures Using Molecular Dynamics Simulation Technique | **J. K. Baria**, P. S. Vyas, A. R. Jivani and A. R. Jani | 2012 | ***American Institute of Physics* CP 1447** (2012) 535 |
| 4 | LASER welding process for RF connectors for space applications | S Srinivasulu, Shivendra Tripathi, R. K. Hegde, **J. K. Baria** | 2018 | ***Int. Journal of emerging Tech. and Advance Engineering (2018) 371*** |

**Papers presented in conferences:**

| Sr No | Title of the paper | Name of Author | Year | Name of the Conference | Date |
|---|---|---|---|---|---|
| 1 | Certain Optical Properties of Gallium Based Semiconductors | P. S. Vyas, J. K. Baria and A. R. Jivani | 2014 | 7th National Level Science symposium 2014 on Recent Trends in Science and Technology, Christ College, Rajkot | 23rd February, 2014 |
| 2 | Some Elastic Properties of $Al_xB_{1-x}N$ Semiconductor Alloys | A. R. Jivani, J. K. Baria, P. S. Vyas and A. R. Jani | 2014 | 7th National Level Science symposium 2014 on Recent Trends in Science and Technology, Christ College, Rajkot | 23rd February, 2014 |
| 3 | Certain physical properties of gallium based semiconductors | P. S. Vyas, J. K. Baria and A. R. Jivani | 2013 | National Conference on Condensed Matter Physics and Applications (CMPA 2013), Department of Physics, Manipal Institute of Technology, Manipal University, Manipal | 27th – 28th December, 2013 |
| 4 | 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 | 2013 | International Conference on Recent Trends in Applied Physics & Material Science (RAM2013), Govt. College of Engineering & Technology, Bikaner | 1st – 2nd February 2013 |